



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 03:52 AM UTC

PDB ID : 6GSM / pdb_00006gsm
EMDB ID : EMD-0057
Title : Structure of a partial yeast 48S preinitiation complex in open conformation.
Authors : Llacer, J.L.; Hussain, T.; Gordiyenko, Y.; Ramakrishnan, V.
Deposited on : 2018-06-14
Resolution : 5.15 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:

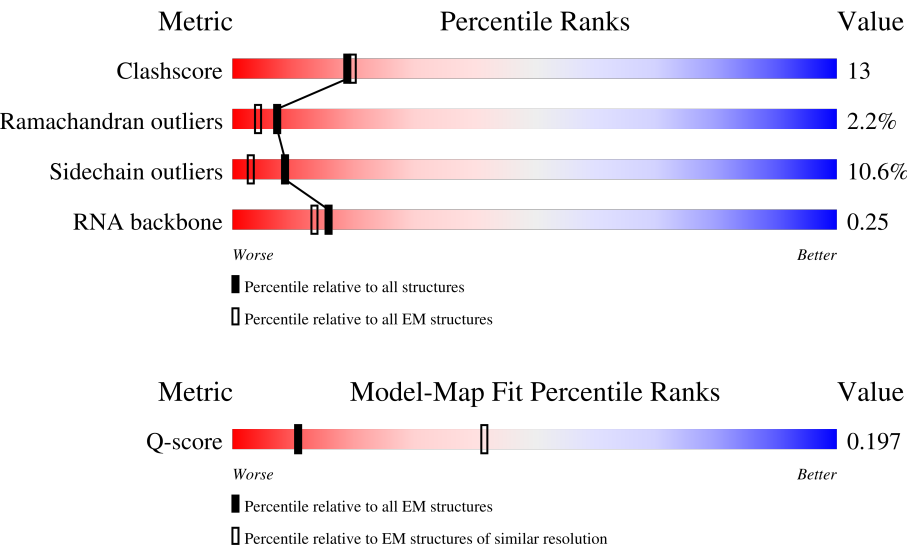
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

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

The reported resolution of this entry is 5.15 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	694 (4.65 - 5.65)

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	1	76	
2	2	1798	
3	A	208	

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Mol	Chain	Length	Quality of chain
4	3	3	100% 100%
5	B	231	38% 66% 24% 6% .
6	C	217	37% 70% 24% 6%
7	D	223	49% 68% 27% 5%
8	E	260	28% 66% 32% .
9	F	206	47% 63% 33% 5%
10	G	226	38% 73% 23% .
11	H	184	43% 61% 28% 10% .
12	I	200	38% 68% 22% . 6%
13	J	182	27% 67% 27% 5%
14	K	96	58% 53% 40% 6% .
15	L	155	39% 79% 18% .
16	M	118	86% 68% 26% 5% .
17	N	150	25% 77% 22% .
18	O	127	28% 77% 20% ..
19	P	119	69% 74% 23% .
20	Q	141	38% 66% 30% .
21	R	125	46% 54% 24% 10% . 11%
22	S	145	51% 58% 37% 6%
23	T	143	36% 71% 27% .
24	U	106	64% 66% 30% .
25	V	87	38% 70% 26% ..
26	W	129	28% 74% 21% ..
27	X	144	41% 60% 32% 8%
28	Y	134	25% 62% 32% 6%

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Mol	Chain	Length	Quality of chain
29	Z	70	
30	a	98	
31	b	81	
32	c	62	
33	d	53	
34	e	58	
35	f	69	
36	g	324	
37	h	25	
38	i	95	
39	j	263	
40	k	430	
41	l	144	
42	m	96	
43	o	567	
44	p	651	
45	q	665	
46	s	342	
47	r	49	

2 Entry composition

There are 51 unique types of molecules in this entry. The entry contains 103158 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called Met-tRNAi.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	74	Total	C	N	O	P	0	0
			1617	724	293	525	75		

- Molecule 2 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	1798	Total	C	N	O	P	0	0
			38175	17061	6721	12595	1798		

- Molecule 3 is a protein called 40S ribosomal protein S0.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	208	Total	C	N	O	S	0	0
			1626	1040	286	298	2		

- Molecule 4 is a RNA chain called mRNA (5'-R(P*AP*AP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	3	Total	C	N	O	P	0	0
			64	29	12	20	3		

- Molecule 5 is a protein called 40S ribosomal protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	222	Total	C	N	O	S	0	0
			1769	1117	324	325	3		

- Molecule 6 is a protein called KLLA0F09812p.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	217	Total	C	N	O	S	0	0
			1629	1041	287	297	4		

- Molecule 7 is a protein called KLLA0D08305p.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	223	Total	C	N	O	S	0	0
			1744	1108	313	318	5		

- Molecule 8 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	260	Total	C	N	O	S	0	0
			2078	1322	393	359	4		

- Molecule 9 is a protein called KLLA0D10659p.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	206	Total	C	N	O	S	0	0
			1609	1008	298	300	3		

- Molecule 10 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	226	Total	C	N	O	S	0	0
			1812	1134	348	326	4		

- Molecule 11 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	184	Total	C	N	O	S	0	0
			1483	950	270	263			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	188	Total	C	N	O	S	0	0
			1489	923	300	265	1		

- Molecule 13 is a protein called KLLA0E23673p.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	182	Total	C	N	O	S	0	0
			1471	929	287	254	1		

- Molecule 14 is a protein called KLLA0B08173p.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	96	Total	C	N	O	S	0	0
			809	533	129	146	1		

- Molecule 15 is a protein called KLLA0A10483p.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	155	Total	C	N	O	S	0	0
			1248	798	237	210	3		

- Molecule 16 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	117	Total	C	N	O	S	0	0
			885	553	161	171			

- Molecule 17 is a protein called KLLA0F18040p.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	150	Total	C	N	O	S	0	0
			1187	756	223	206	2		

- Molecule 18 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	127	Total	C	N	O	S	0	0
			942	578	188	173	3		

- Molecule 19 is a protein called KLLA0F07843p.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	119	Total	C	N	O	S	0	0
			943	604	171	163	5		

- Molecule 20 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	141	Total	C	N	O	S	0	0
			1105	709	204	192			

- Molecule 21 is a protein called KLLA0B01474p.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	R	111	Total	C	N	O	S	0	0
			892	554	165	170	3		

- Molecule 22 is a protein called KLLA0B01562p.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S	145	Total	C	N	O	S	0	0
			1193	741	240	210	2		

- Molecule 23 is a protein called KLLA0A07194p.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	T	143	Total	C	N	O	S	0	0
			1110	693	210	207			

- Molecule 24 is a protein called KLLA0F25542p.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	U	106	Total	C	N	O	S	0	0
			845	540	152	152	1		

- Molecule 25 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	V	87	Total	C	N	O	S	0	0
			687	424	126	135	2		

- Molecule 26 is a protein called 40S ribosomal protein S22.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	W	129	Total	C	N	O	S	0	0
			1021	651	187	180	3		

- Molecule 27 is a protein called KLLA0B11231p.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	X	144	Total	C	N	O	S	0	0
			1119	708	218	191	2		

- Molecule 28 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	Y	134	Total	C	N	O		
			1061	665	207	189	0	0

- Molecule 29 is a protein called KLLA0B06182p.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Z	70	Total	C	N	O	S		
			558	355	104	98	1	0	0

- Molecule 30 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	a	98	Total	C	N	O	S		
			779	480	165	129	5	0	0

- Molecule 31 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	b	81	Total	C	N	O	S		
			609	379	112	113	5	0	0

- Molecule 32 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	c	62	Total	C	N	O	S		
			487	301	97	88	1	0	0

- Molecule 33 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	d	53	Total	C	N	O	S		
			446	280	89	76	1	0	0

- Molecule 34 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	e	58	Total	C	N	O	S		
			463	290	94	78	1	0	0

- Molecule 35 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	f	69	Total	C	N	O	S	0	0
			549	352	102	91	4		

- Molecule 36 is a protein called KLLA0E12277p.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	g	309	Total	C	N	O	S	0	0
			2403	1526	419	453	5		

- Molecule 37 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	h	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	i	95	Total	C	N	O	S	0	0
			765	475	142	143	5		

- Molecule 39 is a protein called Eukaryotic translation initiation factor 2 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	j	249	Total	C	N	O	S	0	0
			2006	1283	333	382	8		

- Molecule 40 is a protein called Eukaryotic translation initiation factor 2 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	k	414	Total	C	N	O	S	0	0
			3123	1985	560	562	16		

- Molecule 41 is a protein called Eukaryotic translation initiation factor 2 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l	130	Total	C	N	O	S	0	0
			1048	669	188	184	7		

- Molecule 42 is a protein called Eukaryotic translation initiation factor eIF-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	m	96	Total	C	N	O	S	0	0
			736	464	134	134	4		

- Molecule 43 is a protein called Eukaryotic translation initiation factor 3 subunit A, Eukaryotic translation initiation factor 3 subunit A, eIF3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	o	528	Total	C	N	O	S	0	0
			4051	2587	695	762	7		

- Molecule 44 is a protein called Eukaryotic translation initiation factor 3 subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	p	651	Total	C	N	O	S	0	0
			5092	3259	881	935	17		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
p	?	-	ALA	deletion	UNP P06103
p	?	-	SER	deletion	UNP P06103
p	?	-	ILE	deletion	UNP P06103
p	?	-	ALA	deletion	UNP P06103
p	?	-	GLN	deletion	UNP P06103
p	?	-	PHE	deletion	UNP P06103
p	?	-	ASP	deletion	UNP P06103
p	?	-	LEU	deletion	UNP P06103
p	?	-	ILE	deletion	UNP P06103
p	?	-	LEU	deletion	UNP P06103

- Molecule 45 is a protein called Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	q	665	Total	C	N	O	S	0	0
			5051	3212	857	970	12		

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
q	?	-	ASP	deletion	UNP P32497
q	?	-	LYS	deletion	UNP P32497
q	?	-	ASN	deletion	UNP P32497

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Chain	Residue	Modelled	Actual	Comment	Reference
q	?	-	PRO	deletion	UNP P32497
q	?	-	GLU	deletion	UNP P32497
q	?	-	SER	deletion	UNP P32497
q	?	-	PHE	deletion	UNP P32497
q	?	-	ASP	deletion	UNP P32497
q	?	-	LYS	deletion	UNP P32497
q	?	-	GLU	deletion	UNP P32497
q	?	-	PRO	deletion	UNP P32497
q	?	-	THR	deletion	UNP P32497
q	?	-	ALA	deletion	UNP P32497
q	?	-	ASP	deletion	UNP P32497
q	?	-	LEU	deletion	UNP P32497
q	?	-	ASP	deletion	UNP P32497
q	?	-	ILE	deletion	UNP P32497
q	?	-	SER	deletion	UNP P32497
q	?	-	ALA	deletion	UNP P32497
q	?	-	ASN	deletion	UNP P32497
q	?	-	GLY	deletion	UNP P32497
q	?	-	PHE	deletion	UNP P32497
q	?	-	THR	deletion	UNP P32497
q	?	-	ILE	deletion	UNP P32497
q	?	-	SER	deletion	UNP P32497
q	?	-	SER	deletion	UNP P32497
q	?	-	SER	deletion	UNP P32497
q	?	-	GLN	deletion	UNP P32497
q	?	-	GLY	deletion	UNP P32497
q	?	-	ASN	deletion	UNP P32497
q	?	-	ASP	deletion	UNP P32497
q	?	-	GLN	deletion	UNP P32497
q	?	-	ALA	deletion	UNP P32497
q	?	-	VAL	deletion	UNP P32497

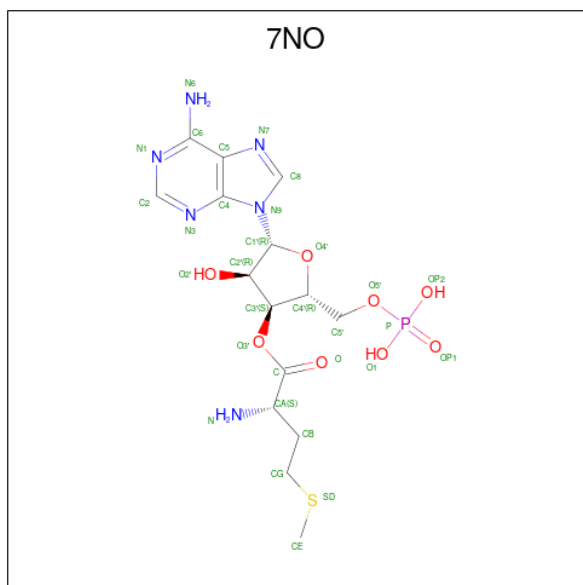
- Molecule 46 is a protein called Eukaryotic translation initiation factor 3 subunit I.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	s	330	Total	C	N	O	S	0	0
			2606	1661	429	507	9		

- Molecule 47 is a protein called Eukaryotic translation initiation factor 3 subunit G.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	r	49	Total	C	N	O	0	0
			392	240	76	76		

- Molecule 48 is [(2 {R},3 {S},4 {R},5 {R})-5-(6-aminopurin-9-yl)-4-oxidanyl-2-(phosphonoxy)methyl)oxolan-3-yl] (2 {S})-2-azanyl-4-methylsulfanyl-butanoate (CCD ID: 7NO) (formula: C₁₅H₂₃N₆O₈PS).



Mol	Chain	Residues	Atoms						AltConf
48	1	1	Total	C	N	O	P	S	0
			30	15	6	7	1	1	

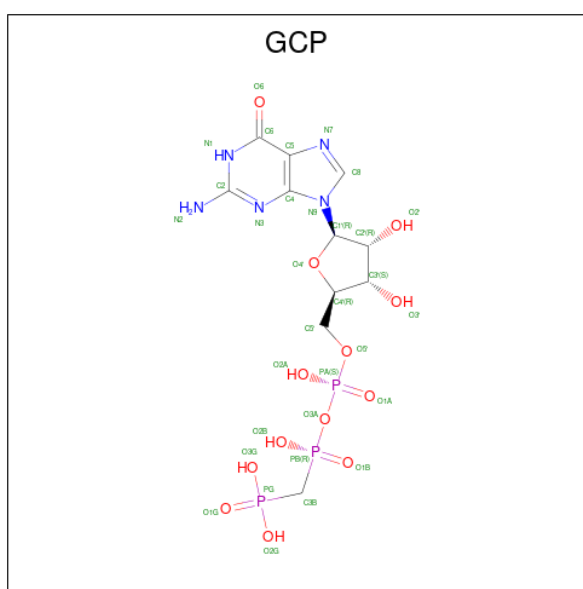
- Molecule 49 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
49	2	76	Total Mg 76 76	0
49	C	3	Total Mg 3 3	0
49	O	1	Total Mg 1 1	0
49	Q	1	Total Mg 1 1	0
49	k	1	Total Mg 1 1	0

- Molecule 50 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
50	O	1	Total	Zn	0
			1	1	
50	b	1	Total	Zn	0
			1	1	
50	f	1	Total	Zn	0
			1	1	
50	l	1	Total	Zn	0
			1	1	

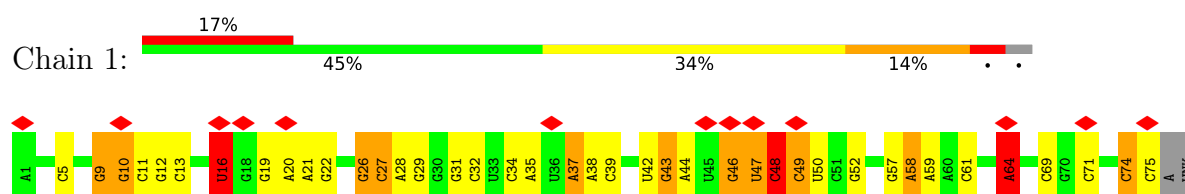
- Molecule 51 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



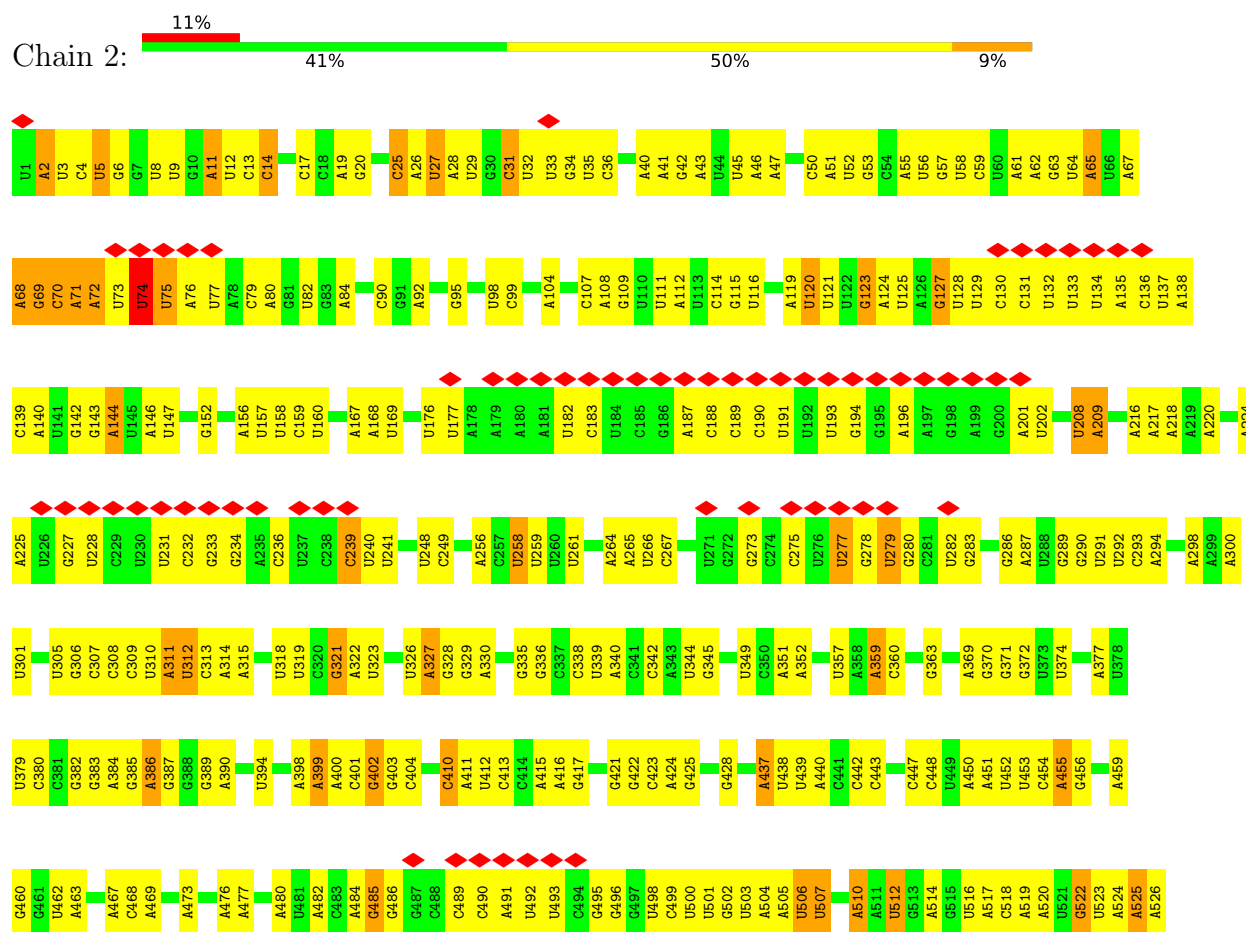
3 Residue-property plots [i](#)

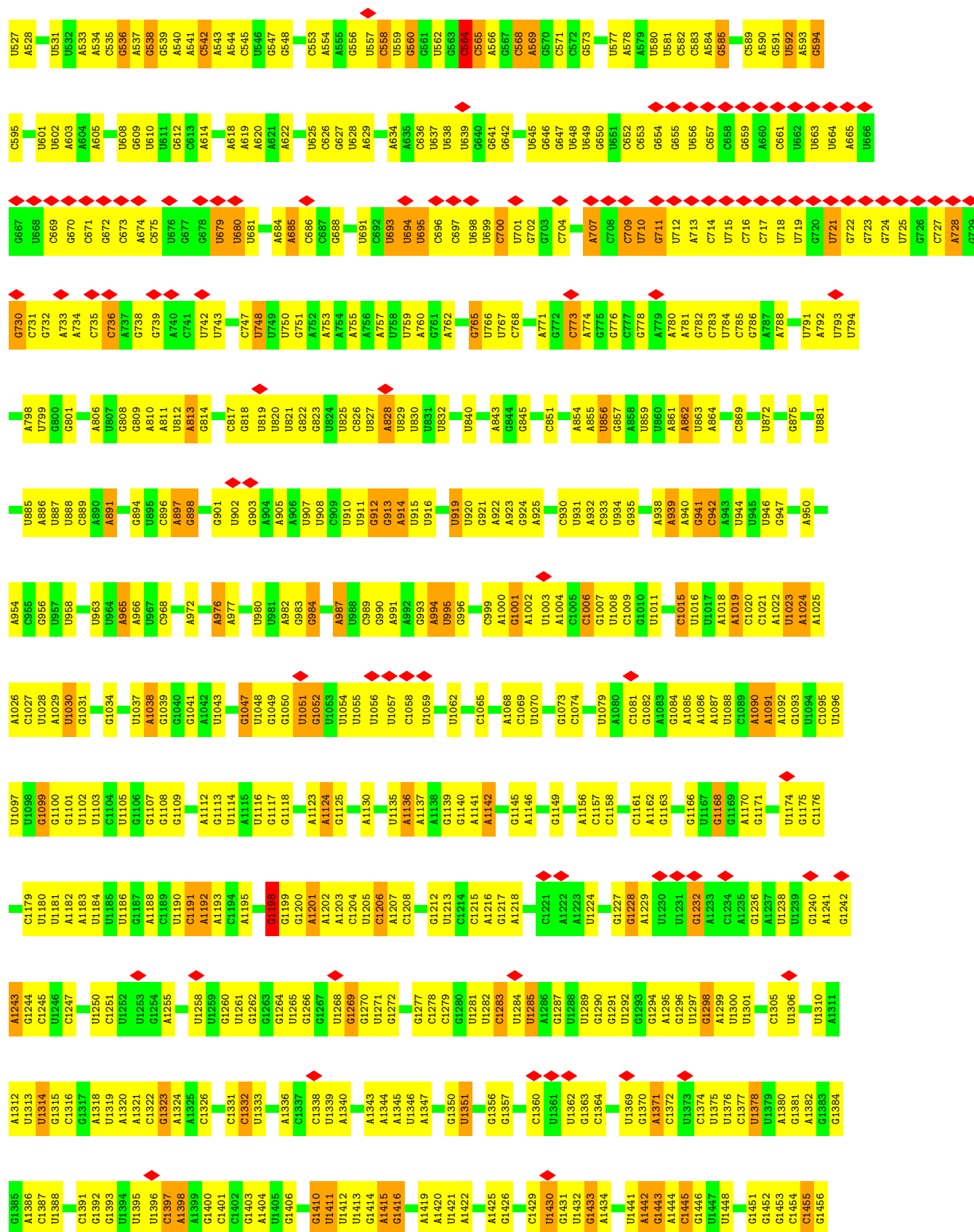
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

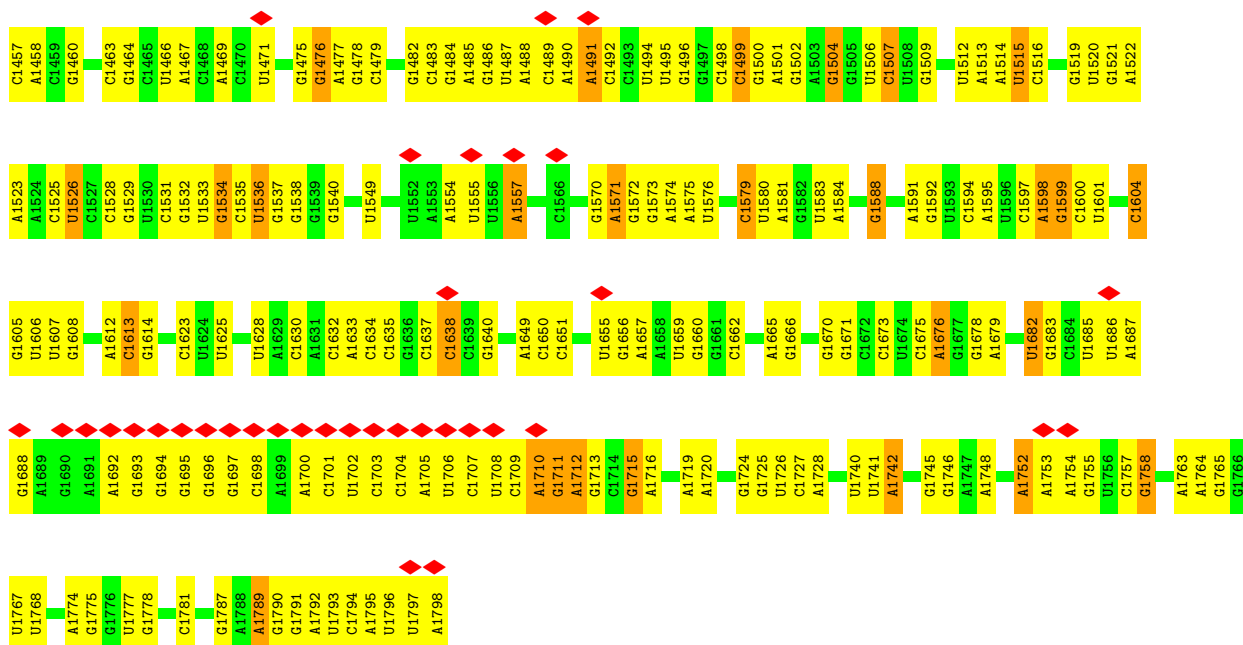
• Molecule 1: Met-tRNAi



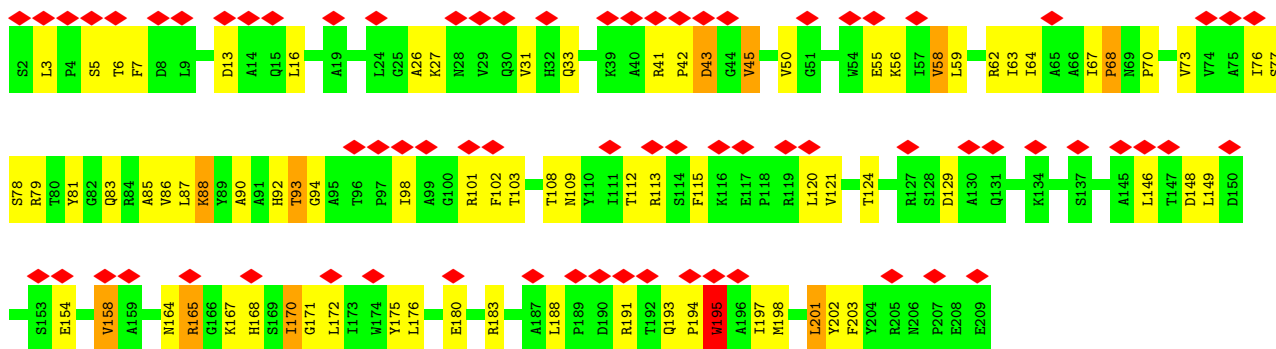
• Molecule 2: 18S ribosomal RNA







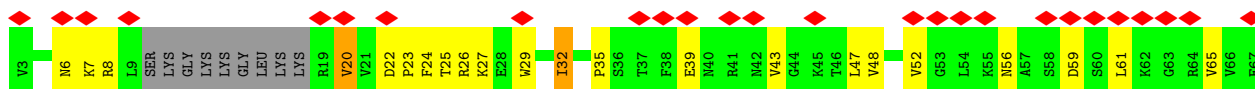
• Molecule 3: 40S ribosomal protein S0

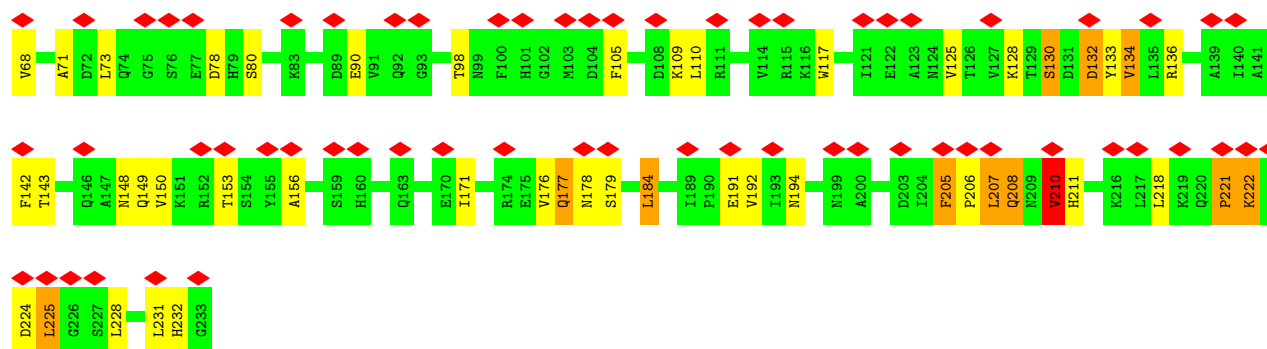


• Molecule 4: mRNA (5'-R(P*AP*AP*U)-3')

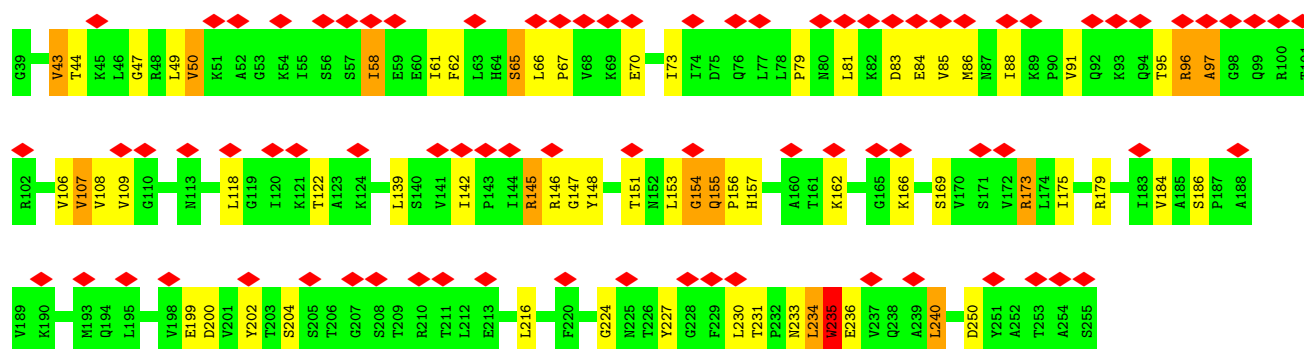


• Molecule 5: 40S ribosomal protein S1

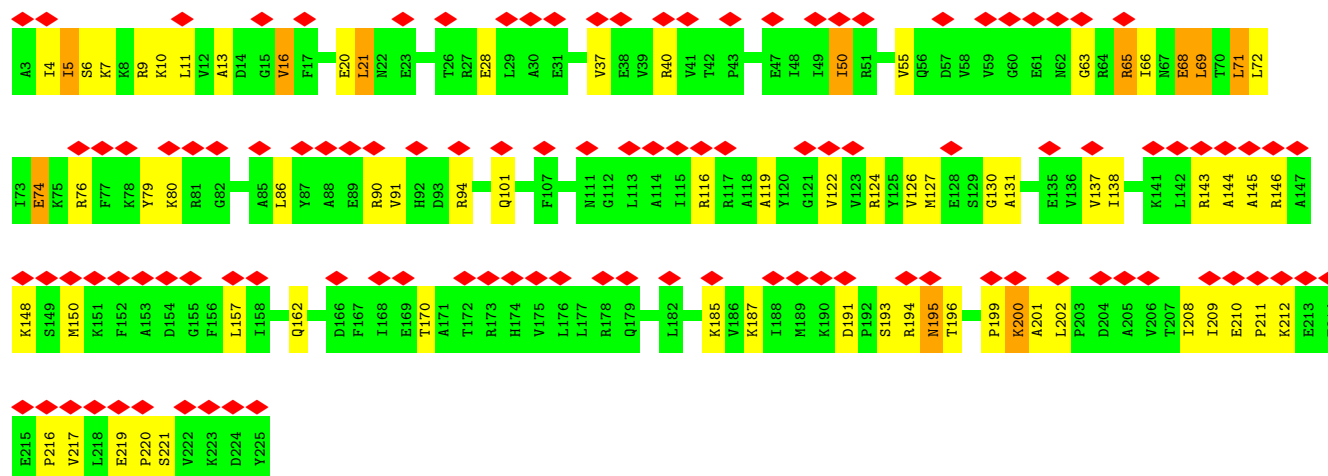




• Molecule 6: KLLA0F09812p

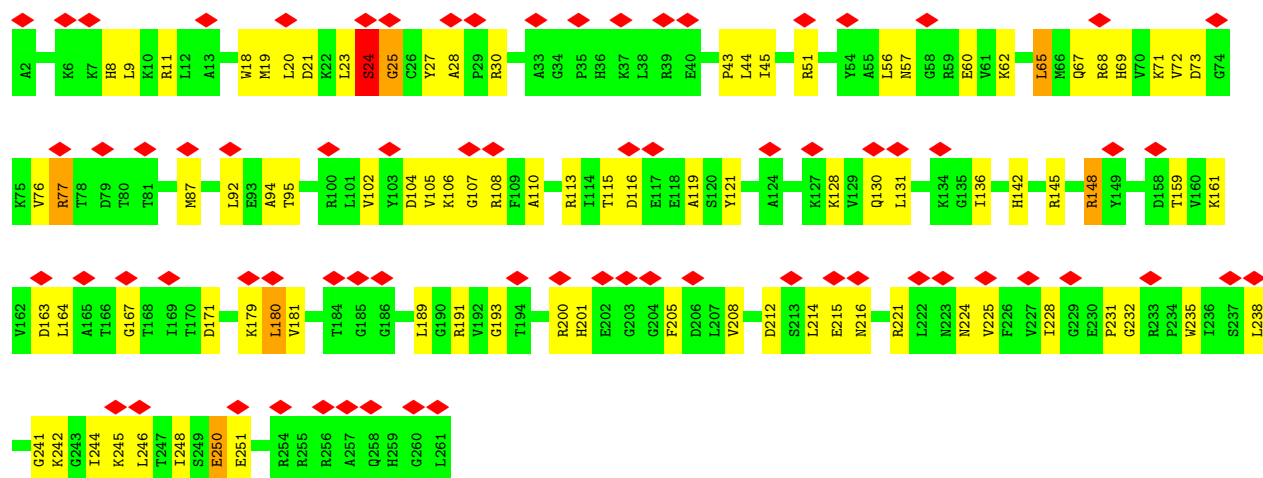


• Molecule 7: KLLA0D08305p

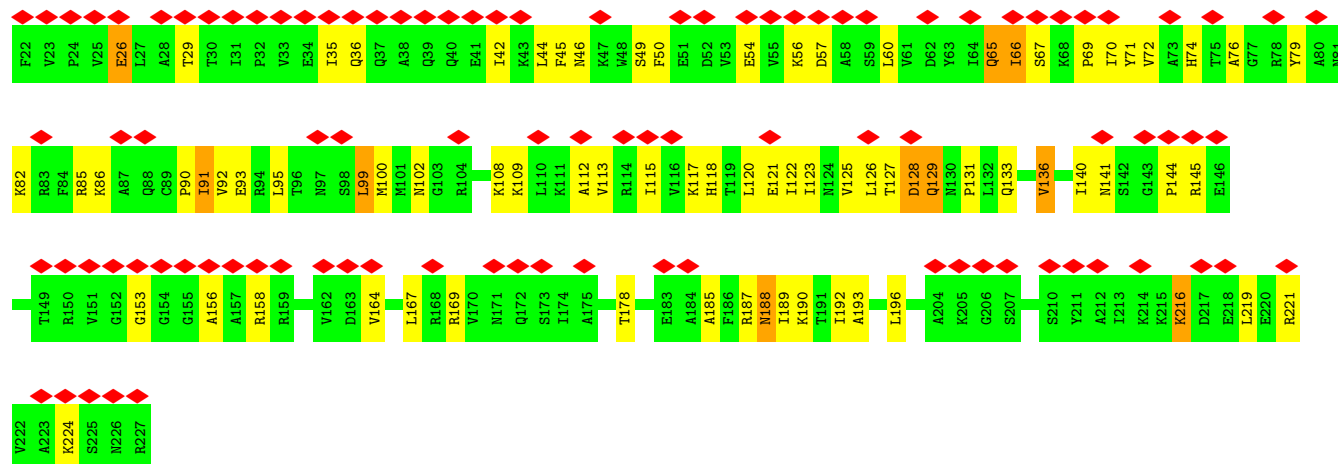


• Molecule 8: 40S ribosomal protein S4

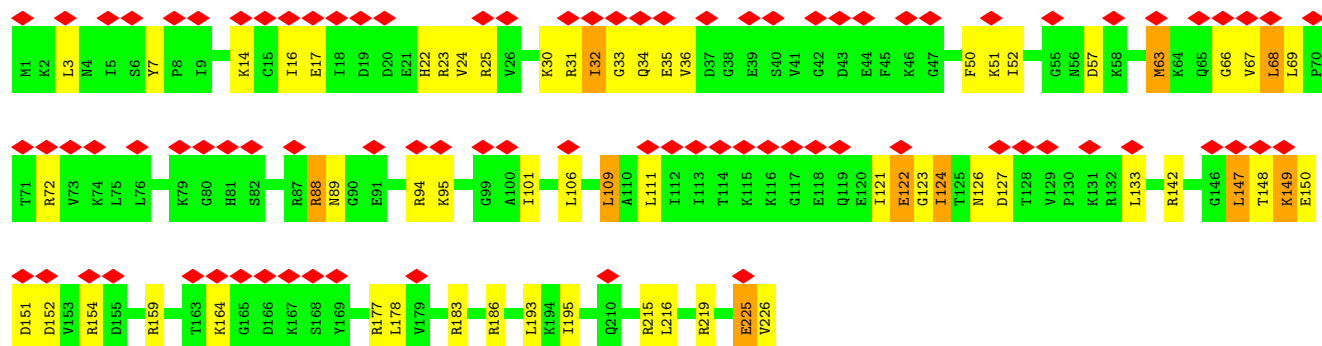
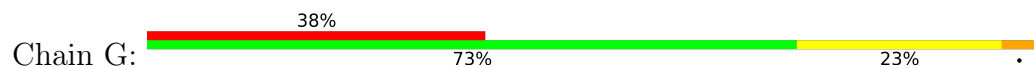




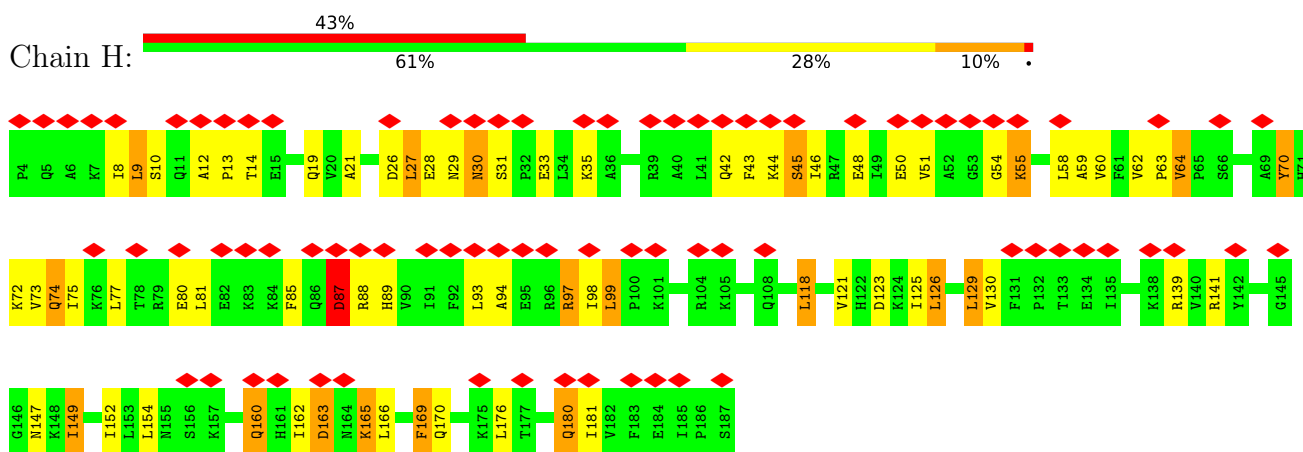
• Molecule 9: KLLA0D10659p



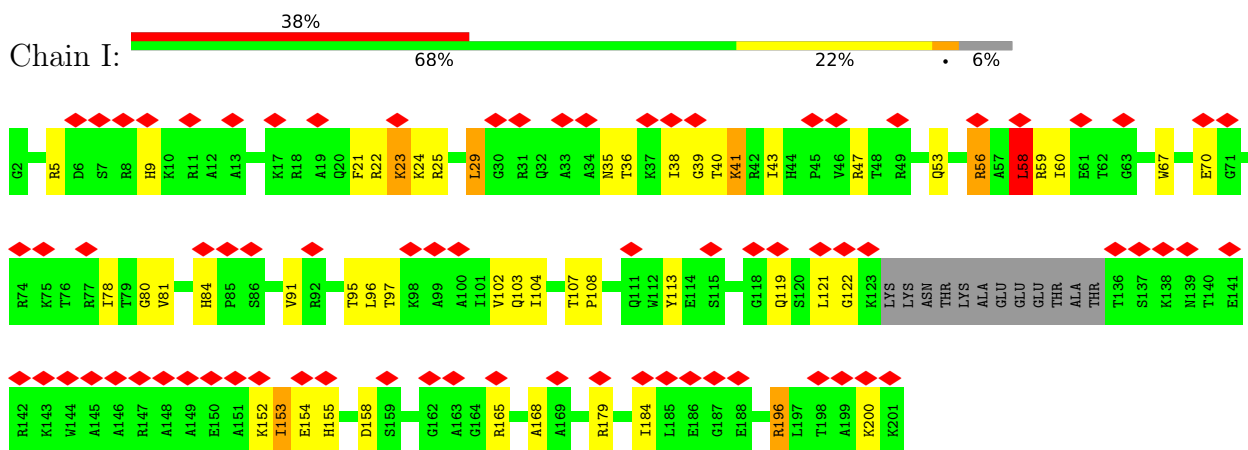
• Molecule 10: 40S ribosomal protein S6



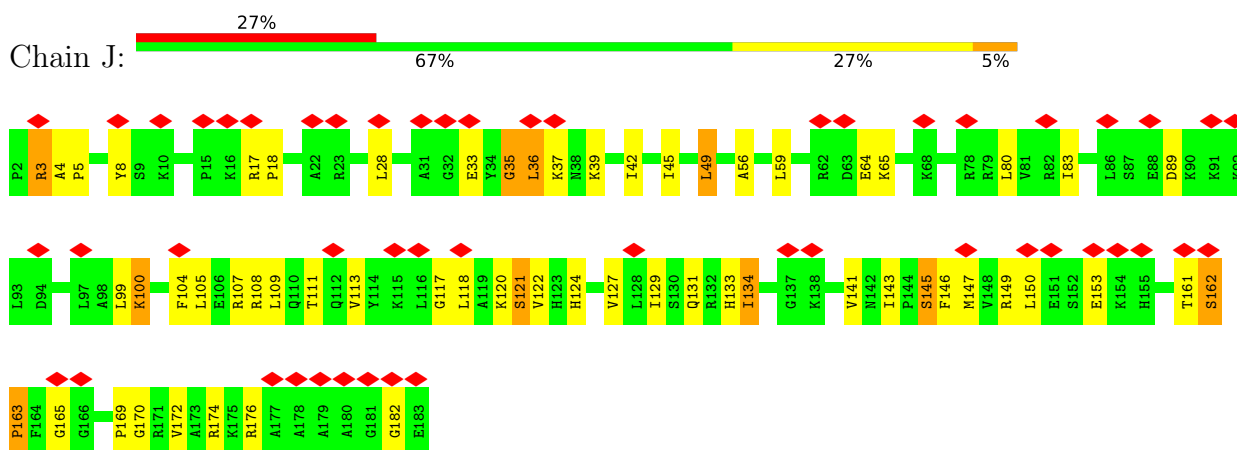
• Molecule 11: 40S ribosomal protein S7



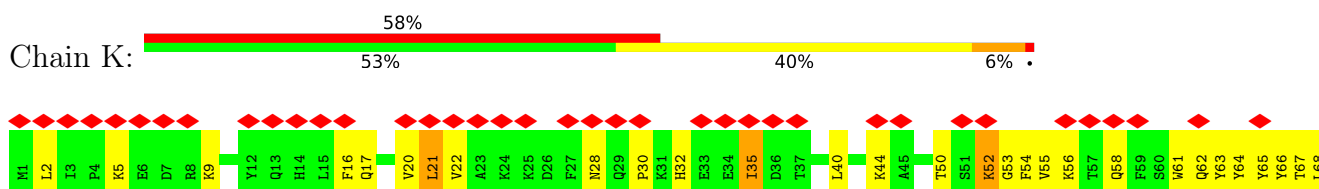
• Molecule 12: 40S ribosomal protein S8

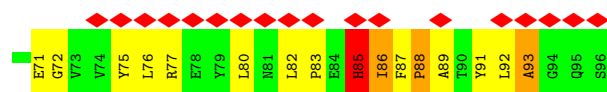


• Molecule 13: KLLA0E23673p

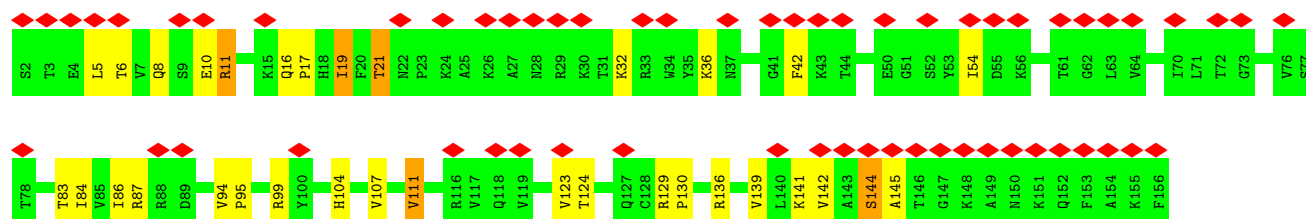
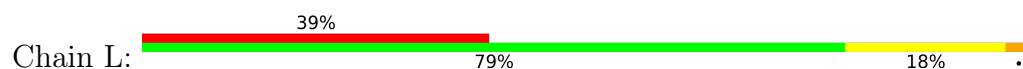


• Molecule 14: KLLA0B08173p

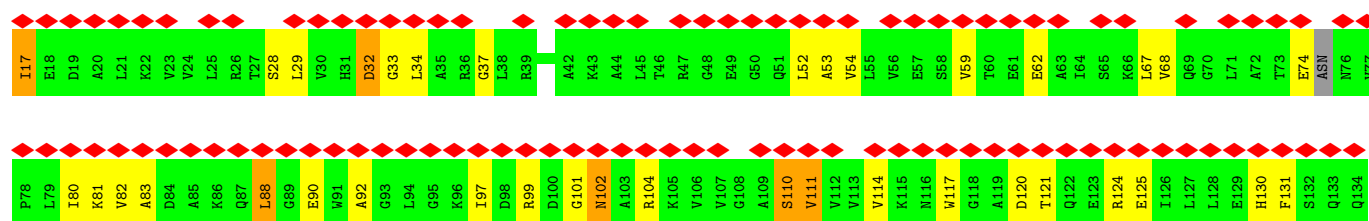
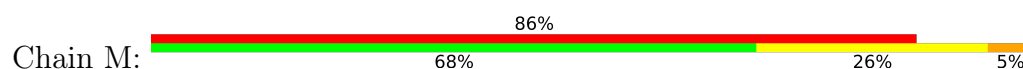




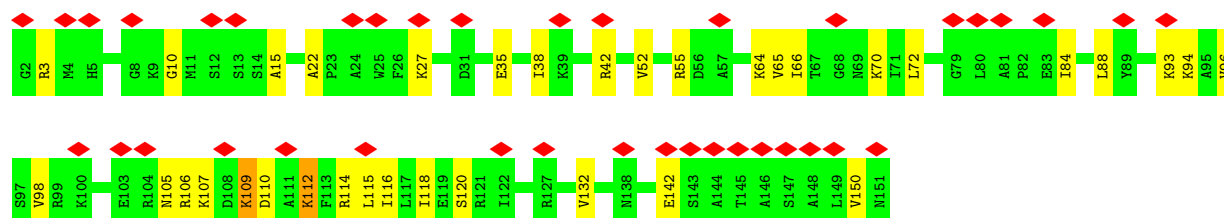
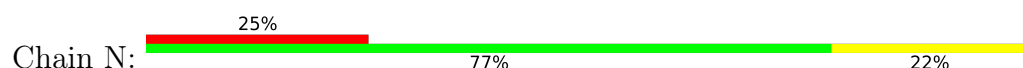
• Molecule 15: KLLA0A10483p



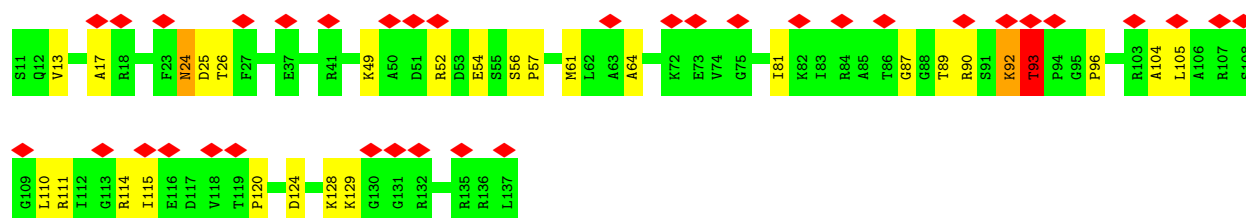
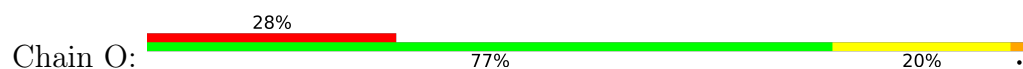
• Molecule 16: 40S ribosomal protein S12



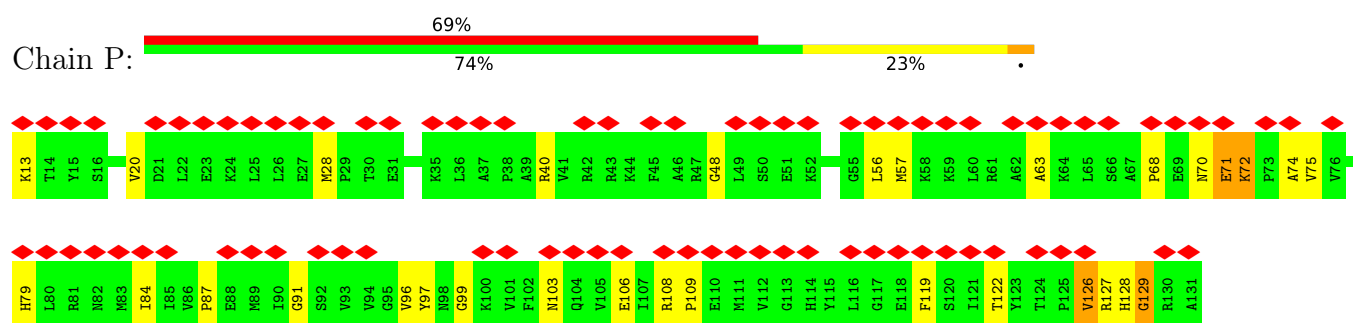
• Molecule 17: KLLA0F18040p



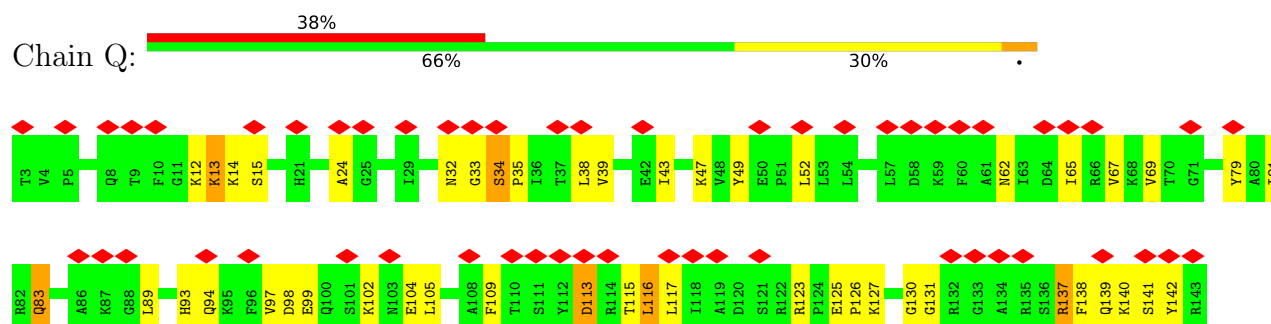
• Molecule 18: 40S ribosomal protein S14



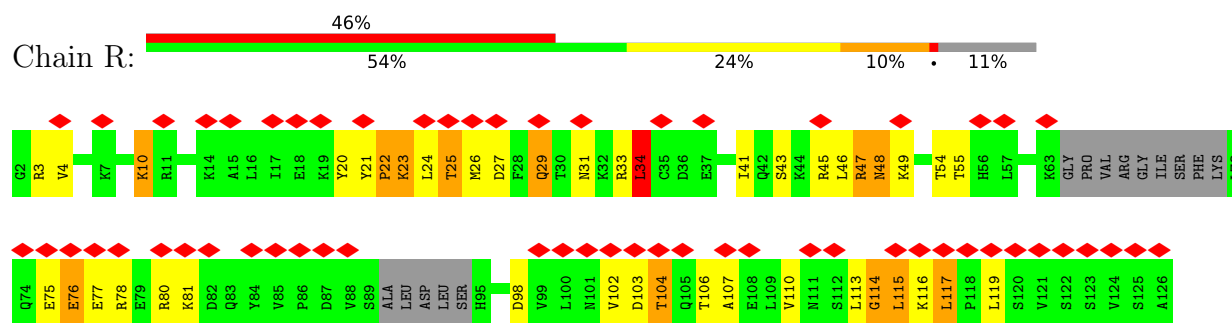
• Molecule 19: KLLA0F07843p



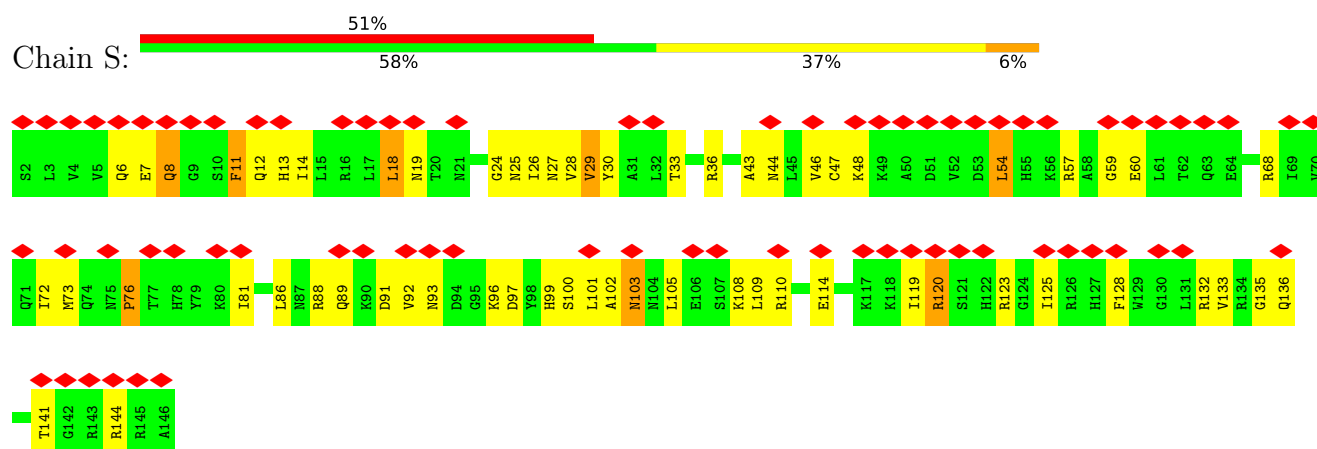
- Molecule 20: 40S ribosomal protein S16



- Molecule 21: KLLA0B01474p

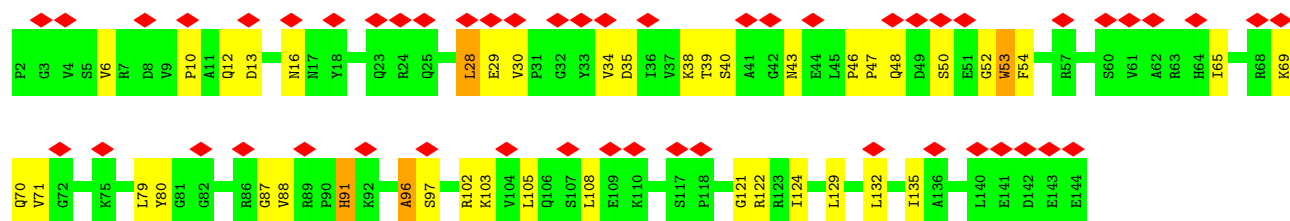


- Molecule 22: KLLA0B01562p

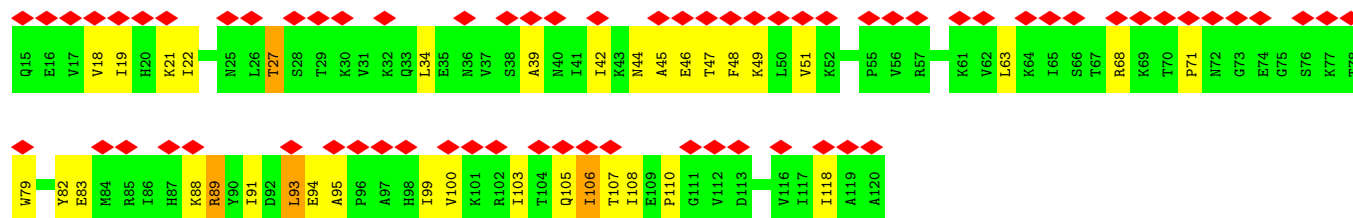


- Molecule 23: KLLA0A07194p

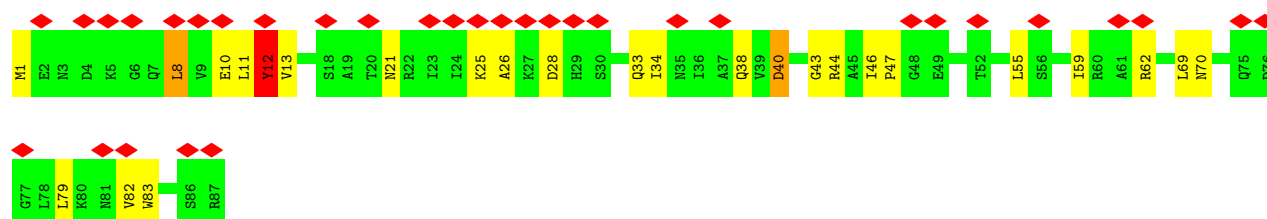
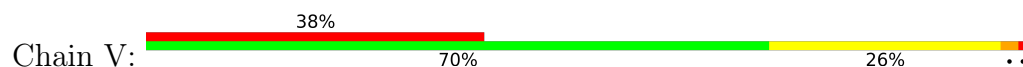




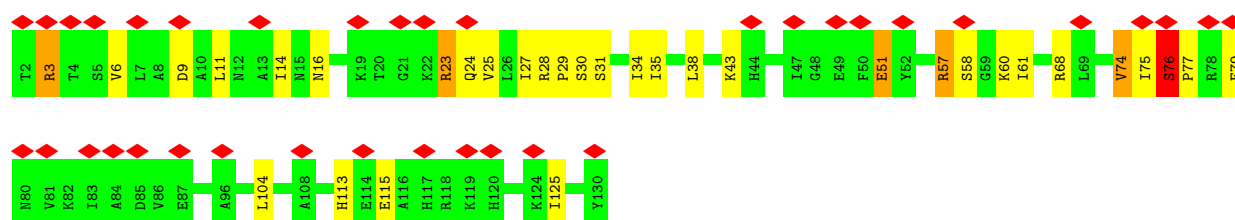
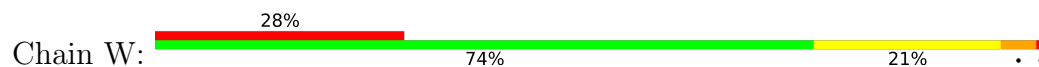
• Molecule 24: KLLA0F25542p



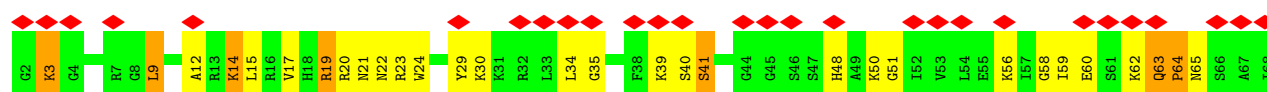
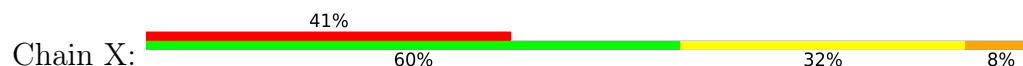
• Molecule 25: 40S ribosomal protein S21

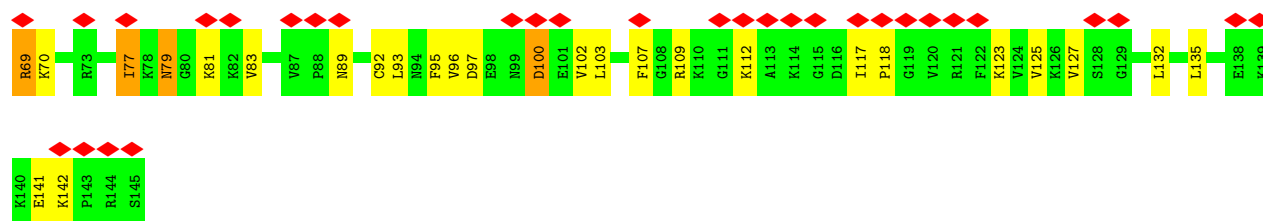


• Molecule 26: 40S ribosomal protein S22

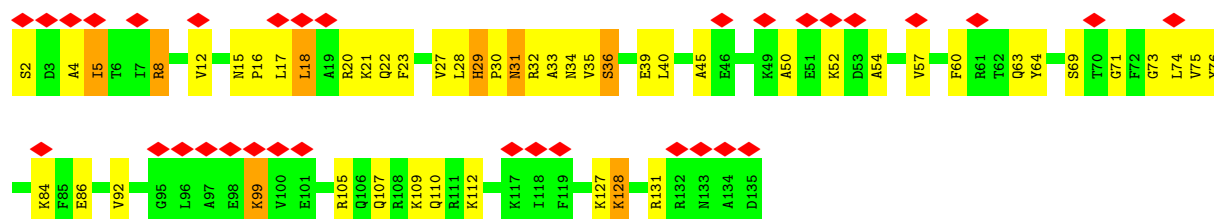


• Molecule 27: KLLA0B11231p

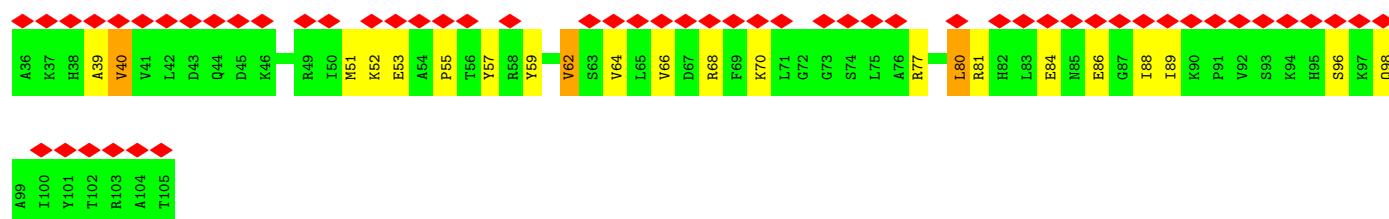
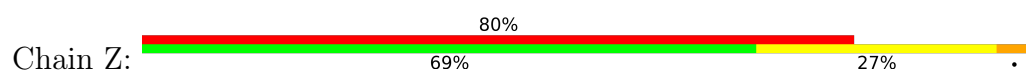




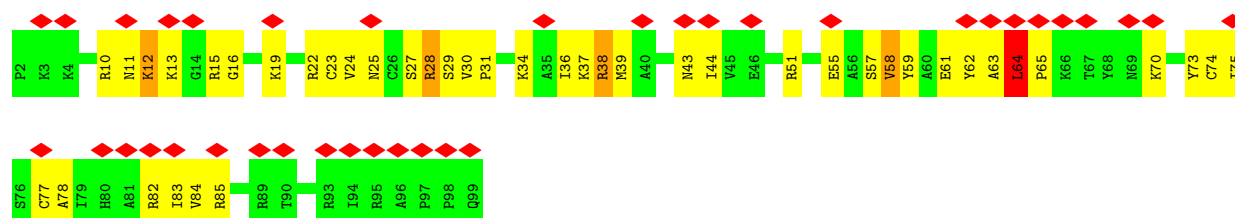
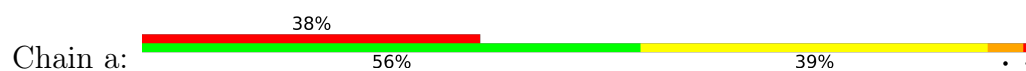
- Molecule 28: 40S ribosomal protein S24



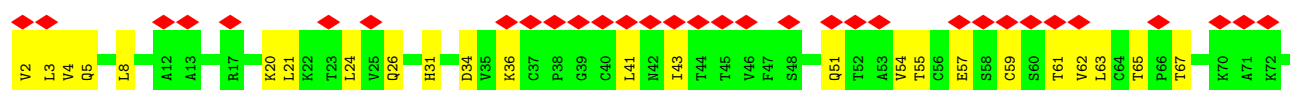
- Molecule 29: KLLA0B06182p

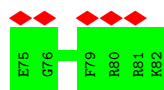


- Molecule 30: 40S ribosomal protein S26

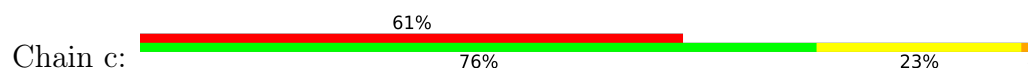


- Molecule 31: 40S ribosomal protein S27





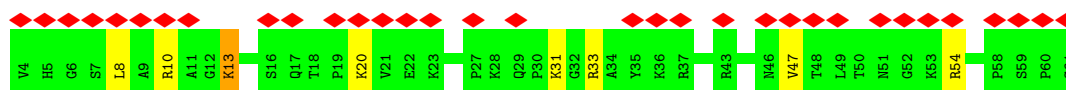
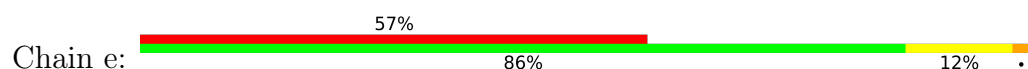
- Molecule 32: 40S ribosomal protein S28



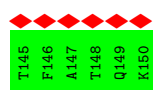
- Molecule 33: 40S ribosomal protein S29



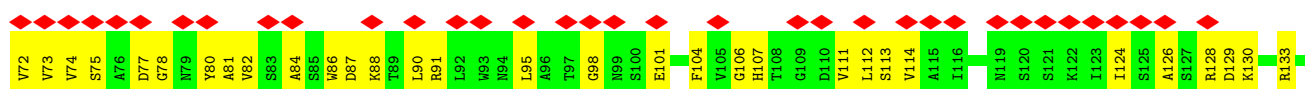
- Molecule 34: 40S ribosomal protein S30

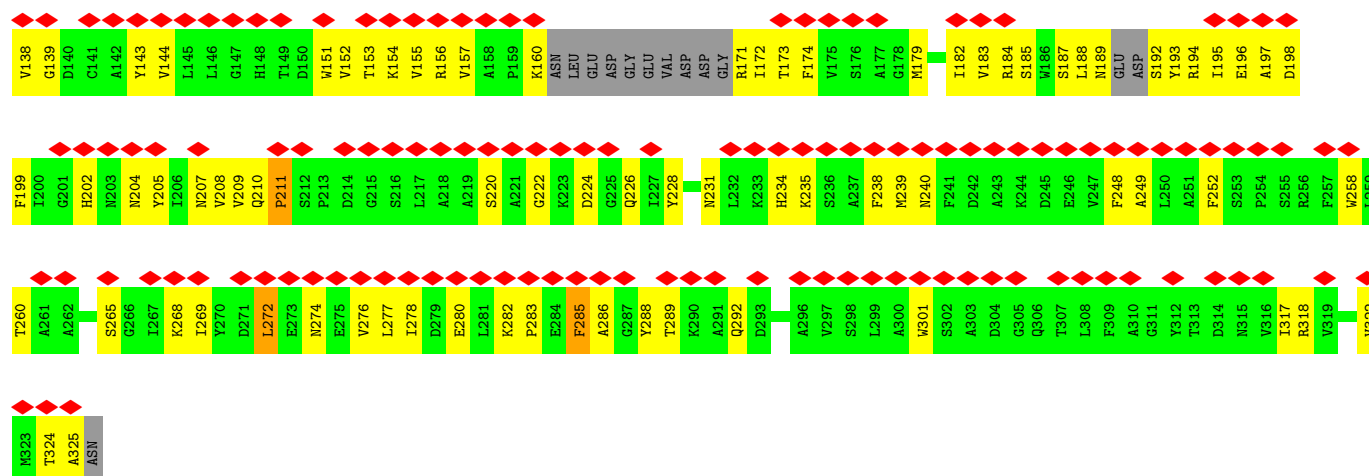


- Molecule 35: Ubiquitin-40S ribosomal protein S27a

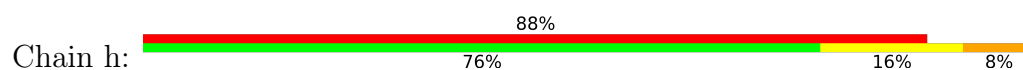


- Molecule 36: KLLA0E12277p

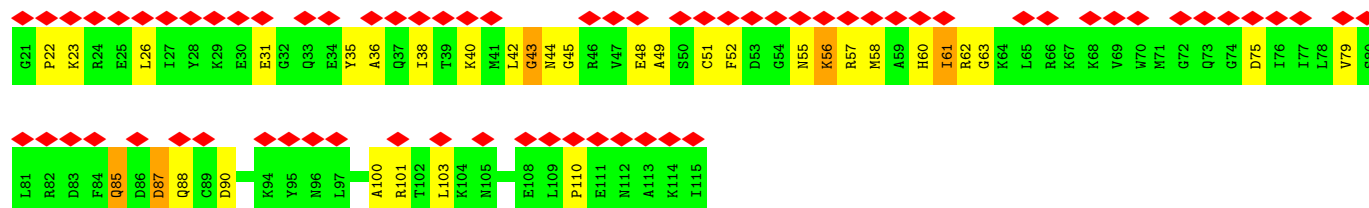
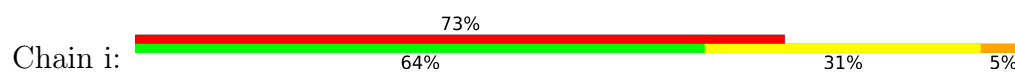




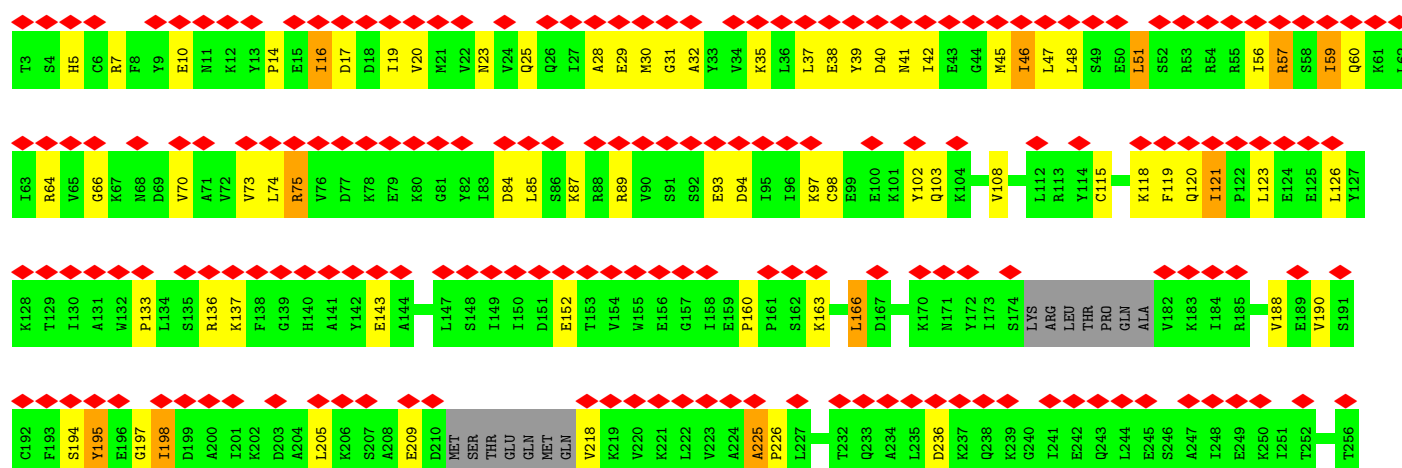
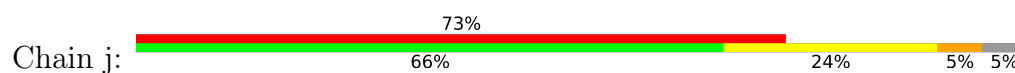
- Molecule 37: 60S ribosomal protein L41-A

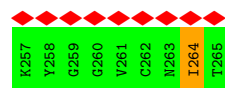


- Molecule 38: Eukaryotic translation initiation factor 1A

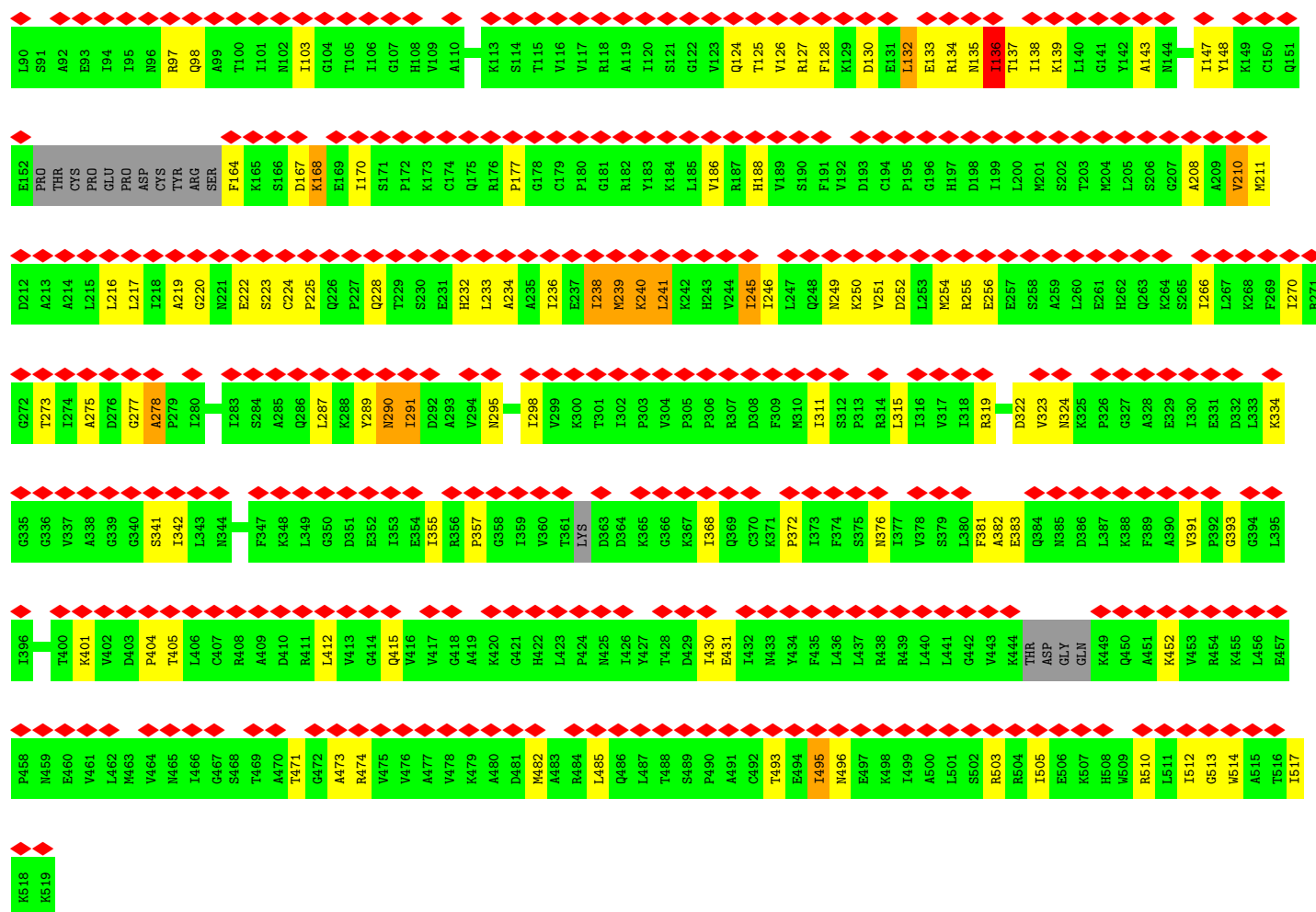
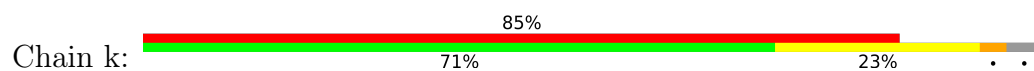


- Molecule 39: Eukaryotic translation initiation factor 2 subunit alpha

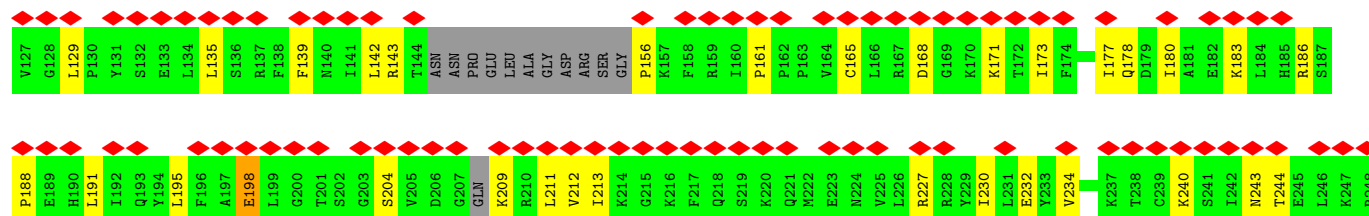


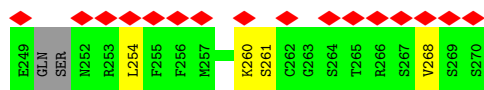


• Molecule 40: Eukaryotic translation initiation factor 2 subunit gamma

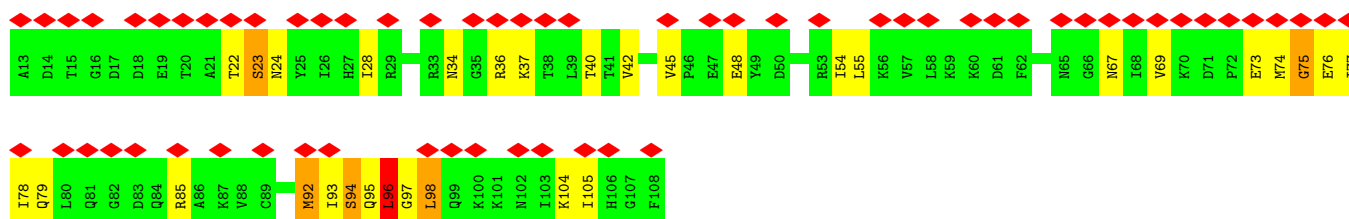


• Molecule 41: Eukaryotic translation initiation factor 2 subunit beta

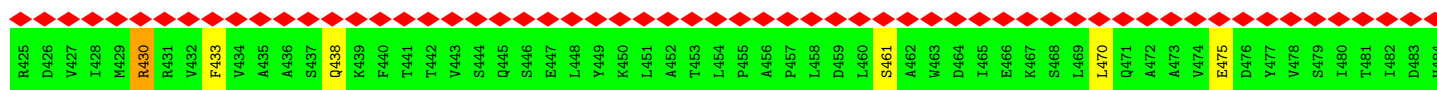
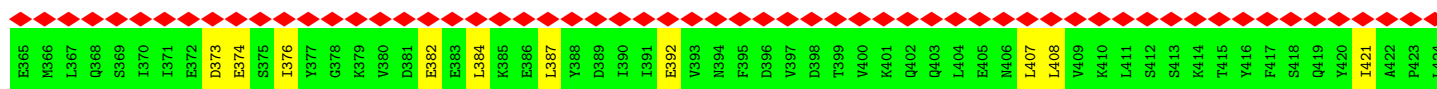
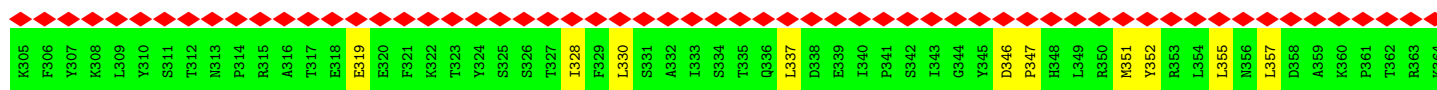
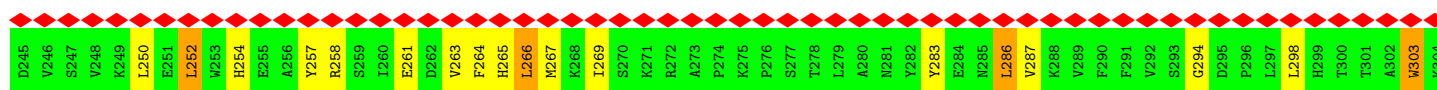
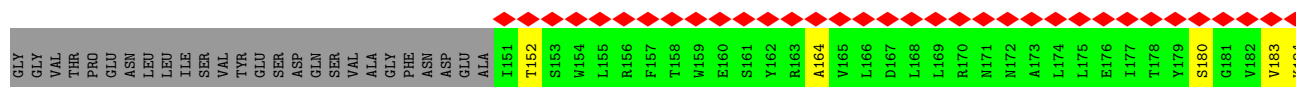
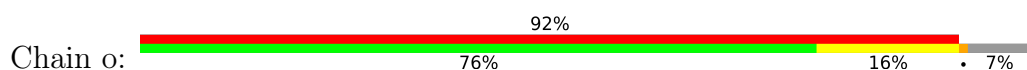


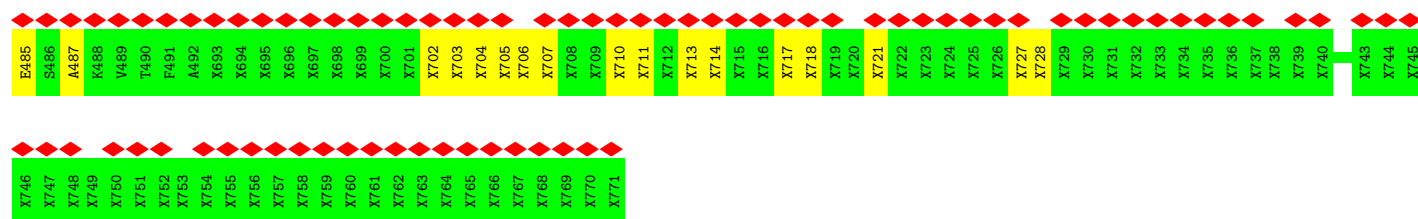


• Molecule 42: Eukaryotic translation initiation factor eIF-1

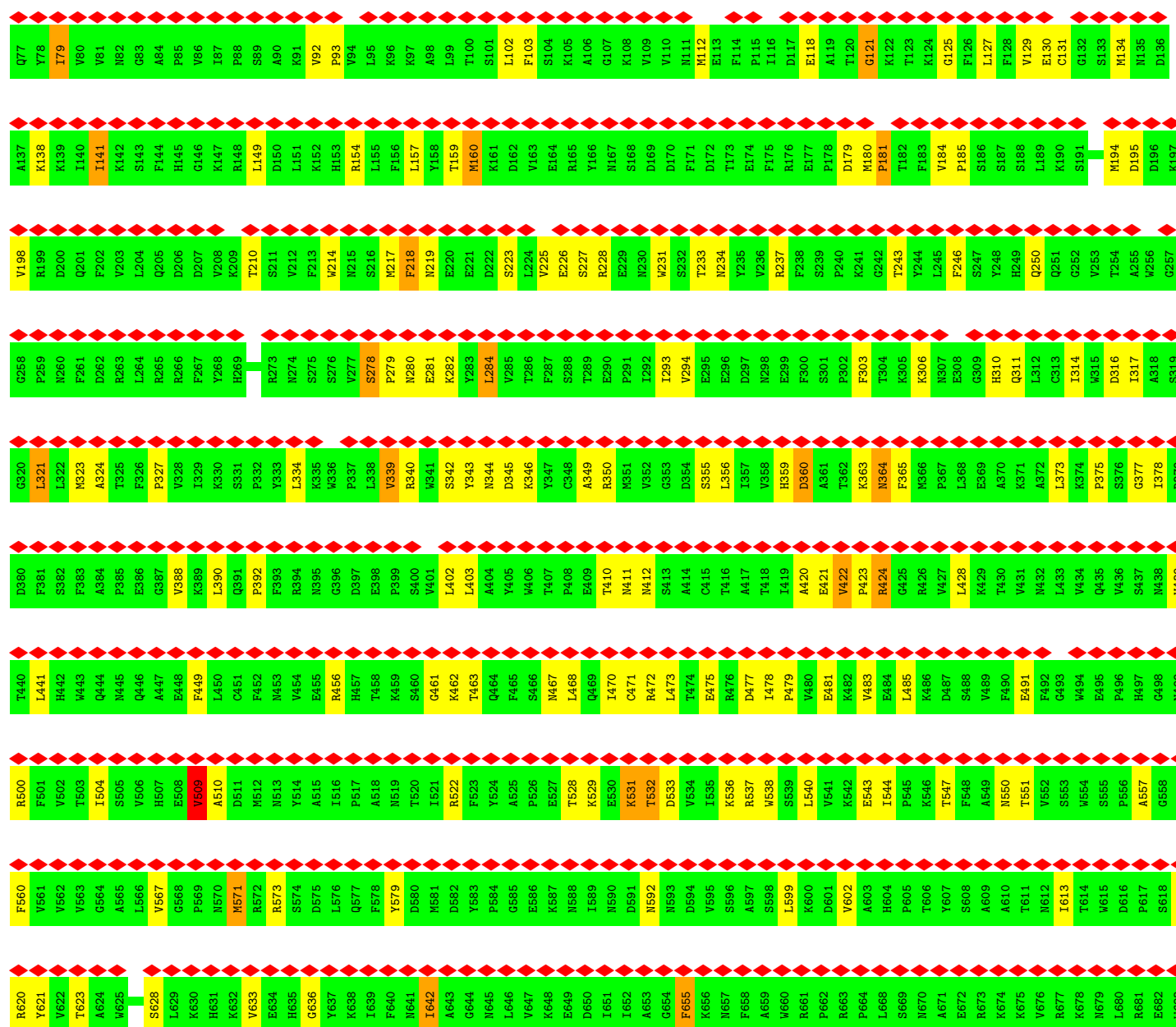
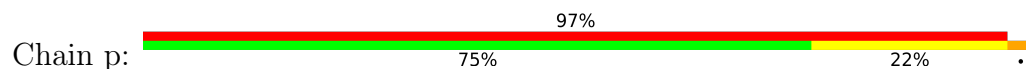


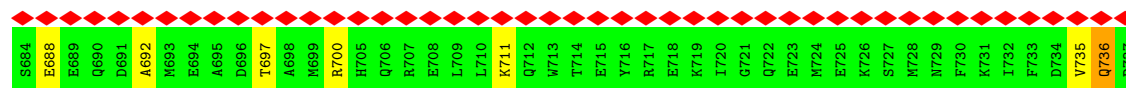
• Molecule 43: Eukaryotic translation initiation factor 3 subunit A, Eukaryotic translation initiation factor 3 subunit A, eIF3a



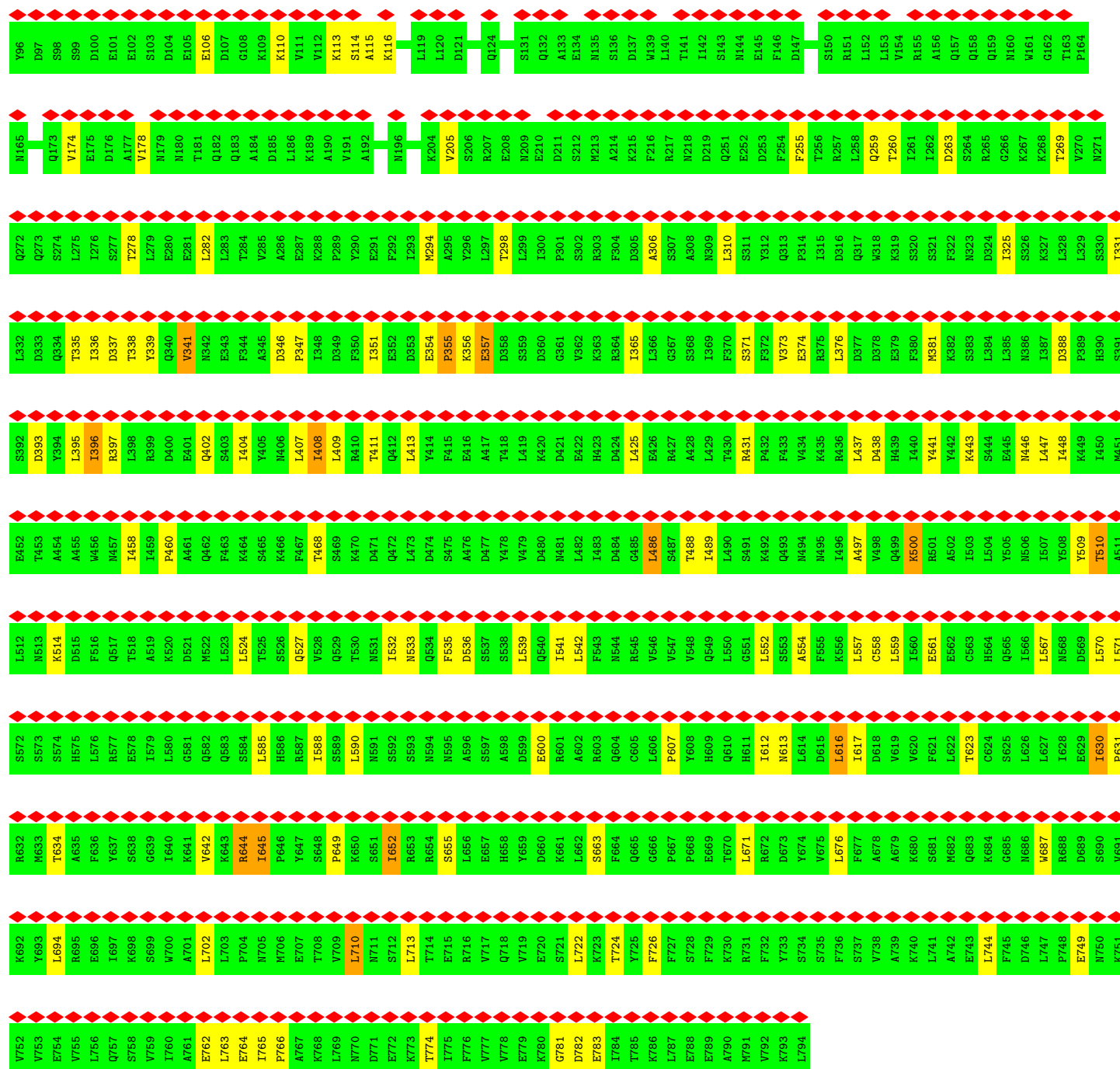
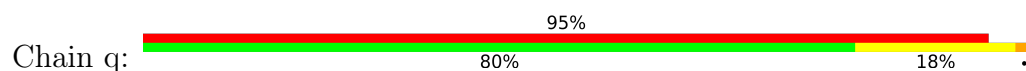


• Molecule 44: Eukaryotic translation initiation factor 3 subunit B





• Molecule 45: Eukaryotic translation initiation factor 3 subunit C



• Molecule 46: Eukaryotic translation initiation factor 3 subunit I

S48	V49	A50	E51	R52	K53	N54	W55	H56	K57	Y58	G59	S60	E61	K62	G63	S64	P65	A66	G67	P68	S69	A70	V71	T72	A73	R74	L75	G76	G77	E78	V79	E80	L81	R82	L83	S84	S85	N86	H87	K88	Q89	A90	E91	E92	E93	R94	I95	C96
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	5750	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.249	Depositor
Minimum map value	-0.118	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	402.0, 402.0, 402.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 1MA, M2G, RIA, 1MG, GCP, T6A, 7NO, 2MG, H2U, 5MC, 7MG, MG, ZN

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	1	0.46	1/1504 (0.1%)	0.78	2/2337 (0.1%)
2	2	0.39	0/42691	0.74	33/66521 (0.0%)
3	A	0.61	0/1666	0.99	0/2279
4	3	0.43	0/71	0.72	0/108
5	B	0.61	0/1793	0.97	1/2414 (0.0%)
6	C	0.59	0/1659	1.03	5/2252 (0.2%)
7	D	0.64	0/1769	0.98	0/2378
8	E	0.57	0/2122	0.94	4/2861 (0.1%)
9	F	0.62	0/1628	1.09	0/2198
10	G	0.56	0/1835	0.92	1/2451 (0.0%)
11	H	0.62	0/1507	1.02	4/2028 (0.2%)
12	I	0.58	0/1515	0.95	2/2029 (0.1%)
13	J	0.55	0/1495	1.08	3/2001 (0.1%)
14	K	0.65	0/831	1.03	2/1123 (0.2%)
15	L	0.61	0/1276	0.90	2/1718 (0.1%)
16	M	0.66	0/891	0.98	1/1201 (0.1%)
17	N	0.55	0/1210	1.07	2/1628 (0.1%)
18	O	0.61	0/953	1.00	1/1279 (0.1%)
19	P	0.70	0/962	0.99	1/1294 (0.1%)
20	Q	0.62	0/1125	1.04	2/1510 (0.1%)
21	R	0.65	0/899	1.06	3/1204 (0.2%)
22	S	0.65	0/1212	1.01	1/1629 (0.1%)
23	T	0.63	0/1129	1.10	2/1520 (0.1%)
24	U	0.63	0/857	1.01	2/1158 (0.2%)
25	V	0.52	0/696	0.93	0/938
26	W	0.55	0/1039	1.00	2/1399 (0.1%)
27	X	0.66	0/1137	1.03	2/1516 (0.1%)
28	Y	0.58	0/1075	1.00	3/1433 (0.2%)
29	Z	0.67	0/567	1.05	1/762 (0.1%)
30	a	0.69	0/791	1.11	6/1059 (0.6%)
31	b	0.60	0/619	0.89	0/837
32	c	0.68	0/489	0.88	0/655

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	d	0.61	0/457	0.88	1/607 (0.2%)
34	e	0.64	0/471	0.95	0/628
35	f	0.81	0/562	1.20	7/751 (0.9%)
36	g	0.40	0/2459	0.74	4/3348 (0.1%)
37	h	0.58	0/234	0.95	0/300
38	i	0.66	0/775	1.02	5/1034 (0.5%)
39	j	0.71	0/2034	0.95	1/2737 (0.0%)
40	k	0.81	1/3168 (0.0%)	0.98	5/4281 (0.1%)
41	l	0.74	0/1064	0.87	0/1420
42	m	0.67	0/744	0.94	1/997 (0.1%)
43	o	0.82	0/3729	0.92	0/5041
44	p	0.78	1/5225 (0.0%)	0.94	4/7101 (0.1%)
45	q	0.82	0/5132	0.96	4/6965 (0.1%)
46	s	0.52	0/2669	0.71	0/3611
47	r	0.43	0/399	0.68	0/535
All	All	0.57	3/108135 (0.0%)	0.87	120/155076 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	k	254	MET	N-CA	5.15	1.52	1.46
1	1	37	T6A	O3'-P	5.12	1.61	1.56
44	p	532	THR	C-O	-5.03	1.17	1.24

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	k	238	ILE	N-CA-C	12.25	122.19	110.30
13	J	161	THR	N-CA-C	11.98	124.08	111.14
40	k	256	GLU	N-CA-C	11.04	123.06	111.14
23	T	53	TRP	N-CA-C	10.54	122.85	111.36
40	k	239	MET	N-CA-C	10.40	122.37	111.14
44	p	280	ASN	N-CA-C	-9.90	91.17	108.69
27	X	3	LYS	N-CA-C	9.62	131.28	110.80
38	i	43	GLY	N-CA-C	9.37	124.77	112.77
2	2	721	U	C2'-C3'-O3'	9.22	123.33	109.50
29	Z	96	SER	N-CA-C	9.03	121.20	111.36
6	C	97	ALA	N-CA-C	8.74	120.42	111.07
11	H	97	ARG	N-CA-C	8.54	120.20	111.07
35	f	87	THR	CA-C-N	8.51	128.13	118.85
35	f	87	THR	C-N-CA	8.51	128.13	118.85
2	2	277	U	C2'-C3'-O3'	8.45	122.17	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	912	G	C2'-C3'-O3'	8.09	121.64	109.50
21	R	104	THR	CB-CA-C	-7.96	107.39	116.54
42	m	92	MET	N-CA-C	7.90	121.86	111.75
2	2	1314	U	C2'-C3'-O3'	7.69	121.04	109.50
16	M	83	ALA	N-CA-C	7.67	119.64	111.28
19	P	126	VAL	N-CA-C	7.61	118.81	109.30
8	E	24	SER	CA-C-N	-7.53	116.53	121.65
8	E	24	SER	C-N-CA	-7.53	116.53	121.65
2	2	1430	U	C2'-C3'-O3'	7.52	120.78	109.50
2	2	1534	G	C4'-C3'-O3'	7.47	120.61	109.40
27	X	69	ARG	N-CA-C	-7.45	97.45	109.96
2	2	239	C	C2'-C3'-O3'	7.10	120.15	109.50
40	k	275	ALA	N-CA-C	7.02	118.72	111.14
44	p	218	PHE	N-CA-C	-7.01	97.79	109.07
2	2	538	G	C4'-C3'-O3'	6.98	119.88	109.40
11	H	99	LEU	N-CA-C	6.95	118.46	109.64
2	2	1030	U	C4'-C3'-O3'	6.84	119.67	109.40
2	2	25	C	C2'-C3'-O3'	6.84	119.76	109.50
23	T	52	GLY	N-CA-C	6.81	122.50	113.37
2	2	1571	A	C4'-C3'-O3'	6.73	119.49	109.40
33	d	35	GLY	N-CA-C	-6.73	105.95	115.30
1	1	74	C	C2'-C3'-O3'	6.70	119.55	109.50
8	E	228	ILE	N-CA-C	6.68	117.76	111.48
30	a	58	VAL	CB-CA-C	-6.65	103.46	111.97
6	C	233	ASN	N-CA-C	6.64	118.52	111.28
20	Q	113	ASP	N-CA-C	6.60	120.48	111.17
21	R	34	LEU	CB-CG-CD2	-6.57	91.00	110.70
8	E	25	GLY	N-CA-C	6.51	122.85	111.46
2	2	828	A	C2'-C3'-O3'	6.51	119.26	109.50
15	L	144	SER	N-CA-C	6.50	118.44	111.36
2	2	1455	C	C4'-C3'-O3'	6.46	119.09	109.40
40	k	254	MET	N-CA-C	6.39	121.12	112.88
2	2	279	U	C2'-C3'-O3'	6.38	119.07	109.50
35	f	120	GLU	N-CA-C	6.36	118.52	108.79
21	R	104	THR	N-CA-C	6.31	117.91	108.31
20	Q	116	LEU	CB-CA-C	-6.28	109.31	116.54
1	1	74	C	C4'-C3'-O3'	6.28	118.82	109.40
2	2	1198	G	C2'-C3'-O3'	6.27	123.11	113.70
2	2	1491	A	C2'-C3'-O3'	6.20	118.80	109.50
44	p	410	THR	N-CA-C	-6.19	105.38	113.12
2	2	1789	A	C4'-C3'-O3'	-6.18	103.73	113.00
2	2	1411	U	C2'-C3'-O3'	6.14	118.72	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	I	58	LEU	N-CA-C	6.10	118.84	111.40
2	2	564	C	C4'-C3'-O3'	5.96	118.34	109.40
18	O	93	THR	N-CA-CB	5.96	120.97	110.37
2	2	1206	C	C4'-C3'-O3'	5.95	118.32	109.40
30	a	19	LYS	CA-C-N	5.94	125.95	119.89
30	a	19	LYS	C-N-CA	5.94	125.95	119.89
2	2	700	C	C2'-C3'-O3'	5.93	122.59	113.70
36	g	285	PHE	N-CA-C	5.87	118.18	108.49
12	I	39	GLY	N-CA-C	-5.82	102.95	110.69
2	2	1430	U	C4'-C3'-O3'	5.81	118.11	109.40
24	U	18	VAL	N-CA-C	5.79	116.57	110.72
22	S	120	ARG	N-CA-C	5.76	119.06	111.28
2	2	1411	U	C4'-C3'-O3'	5.76	118.04	109.40
2	2	1410	G	C2'-C3'-O3'	5.68	118.02	109.50
2	2	828	A	C4'-C3'-O3'	5.66	117.89	109.40
2	2	542	C	C4'-C3'-O3'	5.65	117.88	109.40
30	a	64	LEU	CA-C-N	-5.65	114.14	119.85
30	a	64	LEU	C-N-CA	-5.65	114.14	119.85
14	K	85	HIS	N-CA-C	5.64	117.51	110.91
45	q	533	ASN	N-CA-C	5.64	118.15	111.33
45	q	113	LYS	N-CA-C	5.61	118.37	109.50
2	2	279	U	C4'-C3'-O3'	5.60	117.81	109.40
2	2	258	U	C4'-C3'-O3'	5.60	117.80	109.40
2	2	912	G	C4'-C3'-O3'	5.60	117.79	109.40
2	2	25	C	C4'-C3'-O3'	5.53	117.70	109.40
15	L	11	ARG	N-CA-C	5.51	116.98	110.97
26	W	76	SER	CA-C-N	-5.51	114.57	120.03
26	W	76	SER	C-N-CA	-5.51	114.57	120.03
11	H	99	LEU	CA-C-N	5.50	125.50	120.21
11	H	99	LEU	C-N-CA	5.50	125.50	120.21
6	C	186	SER	CA-C-N	5.50	126.72	119.84
6	C	186	SER	C-N-CA	5.50	126.72	119.84
35	f	110	ASP	N-CA-C	-5.49	100.72	109.23
36	g	52	GLU	CB-CA-C	-5.47	109.78	117.23
24	U	106	ILE	N-CA-C	5.41	116.90	111.00
6	C	235	TRP	N-CA-C	5.40	122.30	110.80
10	G	122	GLU	CB-CA-C	-5.36	110.38	116.54
14	K	52	LYS	N-CA-C	-5.35	105.56	111.71
38	i	87	ASP	N-CA-C	5.33	117.17	111.36
35	f	94	LYS	N-CA-C	5.27	117.66	110.55
2	2	74	U	C4'-C3'-O3'	5.23	117.25	109.40
35	f	105	TYR	N-CA-C	5.23	118.82	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	J	36	LEU	N-CA-C	5.21	116.72	108.96
17	N	84	ILE	CA-C-N	5.21	125.20	119.89
17	N	84	ILE	C-N-CA	5.21	125.20	119.89
28	Y	52	LYS	N-CA-C	5.20	116.95	111.28
5	B	150	VAL	N-CA-C	-5.20	108.43	113.53
2	2	1491	A	C4'-C3'-O3'	5.20	117.20	109.40
28	Y	86	GLU	CA-C-N	5.18	126.31	119.84
28	Y	86	GLU	C-N-CA	5.18	126.31	119.84
35	f	92	ARG	N-CA-C	5.15	119.02	112.12
36	g	286	ALA	CB-CA-C	-5.13	110.64	116.54
45	q	663	SER	N-CA-C	5.12	116.94	111.36
30	a	58	VAL	N-CA-C	5.12	115.33	110.42
13	J	162	SER	N-CA-C	5.10	116.51	108.55
38	i	63	GLY	N-CA-C	5.10	120.24	110.86
2	2	321	G	C4'-C3'-O3'	5.06	116.99	109.40
36	g	211	PRO	CA-N-CD	-5.05	104.93	112.00
44	p	602	VAL	N-CA-C	5.04	115.71	110.82
39	j	194	SER	N-CA-C	5.04	115.96	108.86
38	i	42	LEU	CA-C-N	5.03	125.53	120.00
38	i	42	LEU	C-N-CA	5.03	125.53	120.00
45	q	644	ARG	N-CA-C	5.03	116.46	108.67

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1617	0	841	9	0
2	2	38175	0	19208	307	0
3	A	1626	0	1633	85	0
4	3	64	0	33	0	0
5	B	1769	0	1829	49	0
6	C	1629	0	1710	51	0
7	D	1744	0	1826	35	0
8	E	2078	0	2157	79	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	F	1609	0	1679	49	0
10	G	1812	0	1911	52	0
11	H	1483	0	1579	60	0
12	I	1489	0	1504	52	0
13	J	1471	0	1554	40	0
14	K	809	0	810	75	0
15	L	1248	0	1311	20	0
16	M	885	0	917	31	0
17	N	1187	0	1251	13	0
18	O	942	0	979	13	0
19	P	943	0	989	15	0
20	Q	1105	0	1170	32	0
21	R	892	0	932	50	0
22	S	1193	0	1217	76	0
23	T	1110	0	1124	41	0
24	U	845	0	913	36	0
25	V	687	0	682	34	0
26	W	1021	0	1056	38	0
27	X	1119	0	1198	66	0
28	Y	1061	0	1110	55	0
29	Z	558	0	585	42	0
30	a	779	0	830	72	0
31	b	609	0	631	13	0
32	c	487	0	528	16	0
33	d	446	0	436	35	0
34	e	463	0	503	7	0
35	f	549	0	563	62	0
36	g	2403	0	2352	259	0
37	h	233	0	284	4	0
38	i	765	0	769	40	0
39	j	2006	0	2066	86	0
40	k	3123	0	3235	136	0
41	l	1048	0	1090	19	0
42	m	736	0	744	20	0
43	o	4051	0	3794	30	0
44	p	5092	0	4865	111	0
45	q	5051	0	4764	48	0
46	s	2606	0	2528	0	0
47	r	392	0	382	0	0
48	1	30	0	0	3	0
49	2	76	0	0	0	0
49	C	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	O	1	0	0	0	0
49	Q	1	0	0	0	0
49	k	1	0	0	0	0
50	O	1	0	0	0	0
50	b	1	0	0	0	0
50	f	1	0	0	0	0
50	l	1	0	0	0	0
51	k	32	0	14	6	0
All	All	103158	0	84086	2312	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 13.

All (2312) 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)
36:g:157:VAL:HG22	36:g:174:PHE:CE1	1.10	1.62
27:X:92:CYS:CA	27:X:95:PHE:CD1	1.86	1.56
40:k:128:PHE:CE1	40:k:132:LEU:HD11	1.37	1.55
28:Y:29:HIS:CD2	28:Y:34:ASN:O	1.64	1.50
36:g:154:LYS:NZ	36:g:208:VAL:HB	1.20	1.47
36:g:157:VAL:CG2	36:g:174:PHE:HE1	1.24	1.45
27:X:92:CYS:HA	27:X:95:PHE:CD1	0.92	1.44
36:g:231:ASN:ND2	36:g:234:HIS:HD2	1.15	1.42
22:S:11:PHE:CE2	22:S:57:ARG:NH1	1.92	1.37
36:g:50:GLU:HG2	36:g:55:PHE:CZ	1.59	1.36
40:k:136:ILE:HD12	40:k:137:THR:N	1.39	1.35
8:E:11:ARG:NE	8:E:25:GLY:HA3	1.04	1.34
8:E:11:ARG:HD2	8:E:25:GLY:C	1.53	1.31
38:i:55:ASN:OD1	38:i:57:ARG:NE	1.60	1.30
44:p:228:ARG:HB2	44:p:231:TRP:NE1	1.43	1.30
12:I:41:LYS:HA	12:I:59:ARG:O	1.22	1.30
6:C:157:HIS:NE2	6:C:179:ARG:HG3	1.47	1.29
8:E:11:ARG:HD2	8:E:25:GLY:O	1.17	1.29
36:g:157:VAL:CG2	36:g:174:PHE:CE1	2.01	1.29
38:i:35:TYR:O	38:i:52:PHE:HD2	1.11	1.29
45:q:510:THR:O	45:q:514:LYS:HB2	1.21	1.28
38:i:51:CYS:HB2	38:i:55:ASN:O	1.17	1.28
36:g:231:ASN:HD21	36:g:234:HIS:CD2	1.51	1.28
8:E:11:ARG:NE	8:E:25:GLY:CA	1.95	1.26
9:F:65:GLN:OE1	9:F:90:PRO:HA	1.33	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:g:174:PHE:CE2	36:g:188:LEU:CD1	2.19	1.26
38:i:51:CYS:CB	38:i:55:ASN:O	1.82	1.25
36:g:174:PHE:HE2	36:g:188:LEU:CD1	1.46	1.25
36:g:154:LYS:HZ2	36:g:208:VAL:CB	1.48	1.25
7:D:16:VAL:HG21	33:d:22:ARG:NH1	1.53	1.24
34:e:10:ARG:NH1	34:e:13:LYS:HG2	1.50	1.24
10:G:68:LEU:O	10:G:101:ILE:CD1	1.86	1.23
44:p:228:ARG:CB	44:p:231:TRP:HE1	1.51	1.23
39:j:40:ASP:OD2	39:j:42:ILE:HD12	1.38	1.22
27:X:20:ARG:O	27:X:24:TRP:CD1	1.92	1.22
35:f:97:LYS:O	35:f:99:LYS:HE3	1.38	1.22
36:g:231:ASN:ND2	36:g:234:HIS:CD2	2.04	1.21
3:A:88:LYS:HD3	3:A:202:TYR:CD1	1.74	1.21
5:B:117:TRP:HE3	5:B:153:THR:CG2	1.54	1.20
28:Y:29:HIS:CE1	28:Y:33:ALA:HA	1.75	1.19
21:R:23:LYS:HE3	36:g:205:TYR:OH	1.43	1.19
12:I:36:THR:OG1	12:I:96:LEU:C	1.84	1.19
13:J:121:SER:OG	13:J:124:HIS:CB	1.90	1.18
36:g:154:LYS:NZ	36:g:208:VAL:CB	2.04	1.18
44:p:343:TYR:OH	44:p:346:LYS:HD3	1.41	1.18
22:S:13:HIS:O	22:S:24:GLY:HA3	1.39	1.18
36:g:78:GLY:O	36:g:95:LEU:HD12	1.35	1.18
26:W:30:SER:OG	26:W:61:ILE:HD11	1.43	1.17
40:k:125:THR:HG21	40:k:137:THR:CG2	1.73	1.17
40:k:127:ARG:HD3	40:k:132:LEU:O	1.01	1.17
40:k:128:PHE:CE1	40:k:132:LEU:CD1	2.26	1.17
3:A:92:HIS:CE1	3:A:202:TYR:OH	1.97	1.17
3:A:168:HIS:HA	3:A:203:PHE:CE2	1.80	1.17
27:X:92:CYS:HA	27:X:95:PHE:CE1	1.77	1.17
38:i:35:TYR:O	38:i:52:PHE:CD2	1.96	1.17
35:f:97:LYS:O	35:f:99:LYS:CE	1.94	1.15
40:k:127:ARG:CD	40:k:132:LEU:O	1.94	1.15
2:2:1392:G:P	36:g:292:GLN:HE22	1.70	1.15
28:Y:29:HIS:HE1	28:Y:33:ALA:HA	1.01	1.15
36:g:202:HIS:CE1	36:g:228:TYR:HD2	1.64	1.14
21:R:23:LYS:CE	36:g:205:TYR:OH	1.95	1.14
15:L:87:ARG:NH2	15:L:104:HIS:HB2	1.61	1.14
36:g:124:ILE:HD13	36:g:174:PHE:CD1	1.83	1.14
3:A:88:LYS:HD3	3:A:202:TYR:CE1	1.81	1.13
6:C:147:GLY:O	6:C:156:PRO:HB2	1.47	1.12
36:g:204:ASN:HD22	36:g:224:ASP:HB3	1.13	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:147:GLY:C	6:C:156:PRO:HB2	1.74	1.12
14:K:87:PHE:HD2	14:K:91:TYR:CG	1.66	1.12
24:U:22:ILE:CD1	24:U:100:VAL:HG11	1.80	1.12
33:d:23:ILE:HD13	33:d:46:LYS:NZ	1.63	1.12
12:I:154:GLU:HG2	12:I:155:HIS:H	1.13	1.11
30:a:12:LYS:HA	30:a:15:ARG:HH21	1.12	1.11
39:j:28:ALA:HB3	39:j:31:GLY:C	1.74	1.11
5:B:128:LYS:HE3	5:B:132:ASP:HA	1.13	1.11
8:E:71:LYS:HE2	8:E:76:VAL:HG22	1.21	1.11
8:E:71:LYS:CE	8:E:76:VAL:HG22	1.78	1.11
36:g:204:ASN:ND2	36:g:224:ASP:HB3	1.66	1.11
10:G:68:LEU:O	10:G:101:ILE:HD12	1.43	1.11
36:g:174:PHE:CE2	36:g:188:LEU:HD11	1.84	1.11
21:R:23:LYS:HD3	21:R:34:LEU:HD21	1.31	1.10
21:R:29:GLN:HB3	36:g:86:TRP:CZ3	1.85	1.10
11:H:98:ILE:HG12	11:H:121:VAL:HG11	1.26	1.10
41:l:139:PHE:O	41:l:142:LEU:CD1	1.99	1.10
16:M:52:LEU:HB3	16:M:114:VAL:HB	1.27	1.10
33:d:21:CYS:HB2	33:d:30:LEU:HD11	1.28	1.10
2:2:71:A:H3'	2:2:72:A:H5''	1.11	1.10
35:f:97:LYS:O	35:f:99:LYS:CD	1.99	1.10
40:k:238:ILE:HG23	40:k:514:TRP:CB	1.81	1.10
13:J:121:SER:OG	13:J:124:HIS:HB2	1.51	1.09
39:j:38:GLU:OE1	39:j:102:TYR:CD1	2.05	1.08
3:A:88:LYS:HB3	3:A:202:TYR:CD1	1.87	1.08
36:g:154:LYS:HD2	36:g:208:VAL:CA	1.82	1.08
39:j:119:PHE:HB3	39:j:121:ILE:HD11	1.31	1.08
12:I:36:THR:OG1	12:I:96:LEU:O	1.65	1.07
36:g:157:VAL:HG22	36:g:174:PHE:CD1	1.89	1.07
6:C:157:HIS:CD2	6:C:179:ARG:HG3	1.89	1.07
35:f:98:VAL:HG12	35:f:100:LEU:CD2	1.83	1.07
12:I:36:THR:HG1	12:I:96:LEU:C	1.57	1.06
36:g:174:PHE:HE2	36:g:188:LEU:HD12	0.95	1.06
22:S:11:PHE:HA	22:S:59:GLY:O	1.54	1.05
36:g:78:GLY:O	36:g:95:LEU:CD1	2.03	1.05
36:g:50:GLU:HG2	36:g:55:PHE:CE1	1.91	1.04
41:l:139:PHE:O	41:l:142:LEU:HD12	1.58	1.04
36:g:8:LEU:HD13	36:g:269:ILE:CD1	1.87	1.04
36:g:226:GLN:HB3	36:g:240:ASN:HD21	1.17	1.04
22:S:11:PHE:HE2	22:S:57:ARG:NH1	1.39	1.04
24:U:22:ILE:HD13	24:U:100:VAL:HG11	1.12	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:d:34:TYR:HB2	33:d:36:LEU:HD12	1.38	1.04
35:f:98:VAL:HG12	35:f:100:LEU:HD22	1.34	1.04
28:Y:29:HIS:CD2	28:Y:34:ASN:C	2.27	1.04
35:f:107:LYS:HZ3	35:f:116:LYS:N	1.54	1.03
35:f:107:LYS:HZ1	35:f:116:LYS:C	1.66	1.03
27:X:34:LEU:O	27:X:39:LYS:HE3	1.58	1.03
36:g:202:HIS:CE1	36:g:228:TYR:CD2	2.46	1.03
30:a:36:ILE:HB	30:a:73:TYR:HB2	1.37	1.03
40:k:97:ARG:CB	40:k:186:VAL:O	2.07	1.03
27:X:92:CYS:N	27:X:95:PHE:CE1	2.27	1.02
38:i:60:HIS:HB3	38:i:88:GLN:OE1	1.58	1.02
3:A:81:TYR:HD2	3:A:167:LYS:HG3	1.20	1.02
13:J:121:SER:OG	13:J:124:HIS:HB3	1.58	1.02
14:K:54:PHE:CD2	14:K:72:GLY:HA2	1.95	1.02
35:f:119:LYS:HD3	35:f:120:GLU:H	1.25	1.02
36:g:82:VAL:CG1	36:g:114:VAL:HG21	1.89	1.02
36:g:174:PHE:CE2	36:g:188:LEU:HD12	1.87	1.02
30:a:36:ILE:HD12	30:a:78:ALA:HB2	1.42	1.01
9:F:44:LEU:HD22	9:F:49:SER:HA	1.43	1.01
36:g:81:ALA:HB2	36:g:95:LEU:HD21	1.39	1.01
36:g:209:VAL:HG22	36:g:220:SER:CB	1.90	1.01
39:j:40:ASP:OD2	39:j:42:ILE:CD1	2.09	1.01
40:k:125:THR:HG21	40:k:137:THR:HG21	1.38	1.01
8:E:11:ARG:CD	8:E:25:GLY:C	2.33	1.01
35:f:119:LYS:HA	35:f:119:LYS:HE3	1.41	1.01
7:D:16:VAL:HG21	33:d:22:ARG:HH11	0.84	1.00
12:I:21:PHE:O	12:I:22:ARG:HG3	1.60	1.00
36:g:126:ALA:HB2	36:g:155:VAL:HG13	1.43	1.00
8:E:11:ARG:CZ	8:E:25:GLY:HA3	1.89	1.00
22:S:8:GLN:HA	22:S:11:PHE:CE2	1.97	1.00
45:q:510:THR:O	45:q:514:LYS:CB	2.10	0.99
38:i:55:ASN:OD1	38:i:57:ARG:CZ	2.10	0.99
22:S:12:GLN:OE1	22:S:59:GLY:O	1.78	0.99
35:f:107:LYS:NZ	35:f:116:LYS:N	2.11	0.99
3:A:81:TYR:CD2	3:A:167:LYS:HG3	1.97	0.99
36:g:154:LYS:CD	36:g:208:VAL:HA	1.92	0.99
5:B:117:TRP:CE3	5:B:153:THR:CG2	2.46	0.99
40:k:136:ILE:CD1	40:k:137:THR:N	2.25	0.99
39:j:20:VAL:HA	39:j:39:TYR:CE1	1.97	0.99
22:S:13:HIS:O	22:S:24:GLY:CA	2.11	0.98
14:K:87:PHE:HA	14:K:91:TYR:CE1	1.99	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:71:A:H3'	2:2:72:A:C5'	1.93	0.98
35:f:97:LYS:O	35:f:99:LYS:HD2	1.64	0.98
27:X:92:CYS:CA	27:X:95:PHE:HD1	1.43	0.98
9:F:153:GLY:HA3	9:F:156:ALA:O	1.65	0.97
6:C:157:HIS:NE2	6:C:179:ARG:CG	2.27	0.97
36:g:154:LYS:HD3	36:g:208:VAL:HG23	1.45	0.97
28:Y:29:HIS:CE1	28:Y:33:ALA:CA	2.36	0.97
44:p:314:ILE:CD1	44:p:323:MET:HB2	1.95	0.97
38:i:35:TYR:C	38:i:52:PHE:CD2	2.42	0.97
9:F:65:GLN:OE1	9:F:90:PRO:CA	2.11	0.97
6:C:227:TYR:OH	25:V:11:LEU:HD11	1.65	0.96
40:k:323:VAL:O	40:k:334:LYS:HG3	1.65	0.96
40:k:128:PHE:HE1	40:k:132:LEU:HD11	1.28	0.96
28:Y:5:ILE:HG23	28:Y:28:LEU:O	1.66	0.96
7:D:16:VAL:CG2	33:d:22:ARG:HH11	1.79	0.96
8:E:11:ARG:CD	8:E:25:GLY:O	2.12	0.96
30:a:36:ILE:CD1	30:a:78:ALA:CB	2.43	0.96
36:g:154:LYS:HD2	36:g:208:VAL:HA	0.96	0.96
3:A:81:TYR:HD2	3:A:167:LYS:CG	1.79	0.96
8:E:11:ARG:CD	8:E:25:GLY:CA	2.44	0.96
14:K:64:TYR:O	14:K:66:TYR:CD2	2.19	0.96
40:k:128:PHE:CD1	40:k:132:LEU:CD1	2.49	0.96
3:A:88:LYS:CB	3:A:202:TYR:CD1	2.49	0.95
12:I:41:LYS:HD3	12:I:43:ILE:HD11	1.48	0.95
14:K:16:PHE:O	14:K:88:PRO:HB3	1.66	0.95
27:X:92:CYS:CA	27:X:95:PHE:CE1	2.38	0.95
29:Z:57:TYR:CE2	29:Z:59:TYR:HB3	2.01	0.95
29:Z:57:TYR:HE2	29:Z:59:TYR:HB3	1.25	0.95
36:g:82:VAL:HG11	36:g:114:VAL:HG21	1.46	0.95
30:a:43:ASN:OD1	30:a:64:LEU:HD21	1.67	0.95
30:a:59:TYR:HE1	30:a:62:TYR:HB2	1.32	0.95
39:j:57:ARG:H	39:j:57:ARG:HD2	1.28	0.95
40:k:127:ARG:HD3	40:k:132:LEU:C	1.90	0.95
13:J:121:SER:HG	13:J:124:HIS:HB3	1.31	0.95
14:K:64:TYR:HB3	14:K:66:TYR:CE2	2.01	0.95
40:k:238:ILE:HG23	40:k:514:TRP:HB3	1.45	0.94
12:I:41:LYS:CA	12:I:59:ARG:O	2.14	0.94
40:k:238:ILE:HG23	40:k:514:TRP:HB2	1.48	0.94
13:J:35:GLY:HA3	13:J:122:VAL:CG1	1.96	0.94
26:W:30:SER:HB2	26:W:61:ILE:HG13	1.49	0.94
44:p:509:VAL:HG13	44:p:510:ALA:H	1.30	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:105:VAL:CG1	8:E:244:ILE:O	2.15	0.93
5:B:128:LYS:HE3	5:B:132:ASP:CA	1.98	0.93
7:D:195:ASN:ND2	7:D:199:PRO:O	1.99	0.93
27:X:92:CYS:H	27:X:95:PHE:HE1	1.04	0.93
40:k:238:ILE:CG2	40:k:514:TRP:HB3	1.98	0.93
36:g:106:GLY:O	36:g:133:ARG:NH2	1.80	0.93
26:W:30:SER:OG	26:W:61:ILE:CD1	2.14	0.93
8:E:105:VAL:HG12	8:E:244:ILE:O	1.69	0.93
11:H:98:ILE:CG1	11:H:121:VAL:HG11	1.99	0.93
14:K:87:PHE:CD2	14:K:91:TYR:CG	2.57	0.93
8:E:11:ARG:CD	8:E:25:GLY:HA3	1.97	0.92
36:g:50:GLU:CG	36:g:55:PHE:CZ	2.50	0.92
40:k:136:ILE:HA	51:k:602:GCP:H3B1	1.49	0.92
40:k:232:HIS:O	40:k:236:ILE:HG13	1.67	0.92
14:K:54:PHE:HD2	14:K:72:GLY:HA2	1.34	0.92
22:S:8:GLN:HA	22:S:11:PHE:CD2	2.03	0.92
29:Z:68:ARG:NH2	29:Z:70:LYS:HG3	1.83	0.92
24:U:105:GLN:O	24:U:108:ILE:HD11	1.69	0.92
40:k:128:PHE:CD1	40:k:132:LEU:HD11	2.05	0.92
36:g:8:LEU:CD1	36:g:269:ILE:CD1	2.48	0.92
20:Q:13:LYS:HG2	20:Q:79:TYR:HB3	1.52	0.91
36:g:209:VAL:HG22	36:g:220:SER:HB3	1.50	0.91
32:c:13:ILE:HG23	32:c:14:LYS:HD2	1.52	0.91
44:p:316:ASP:OD1	44:p:323:MET:HE2	1.69	0.91
38:i:60:HIS:CB	38:i:88:GLN:OE1	2.17	0.91
25:V:10:GLU:O	25:V:11:LEU:CD1	2.19	0.91
36:g:47:ARG:CD	36:g:59:VAL:HG11	2.01	0.91
40:k:136:ILE:HD12	40:k:137:THR:CA	2.00	0.91
3:A:88:LYS:CD	3:A:202:TYR:CD1	2.54	0.91
21:R:102:VAL:HG13	21:R:119:LEU:HD22	1.49	0.90
38:i:35:TYR:C	38:i:52:PHE:HD2	1.76	0.90
42:m:22:THR:O	42:m:24:ASN:N	2.04	0.90
30:a:36:ILE:HB	30:a:73:TYR:CB	2.00	0.90
36:g:184:ARG:NH1	36:g:198:ASP:OD1	2.04	0.90
5:B:117:TRP:HE3	5:B:153:THR:HG22	1.34	0.90
32:c:13:ILE:HG23	32:c:14:LYS:CD	2.01	0.90
3:A:168:HIS:HA	3:A:203:PHE:CZ	2.07	0.90
23:T:47:PRO:CB	23:T:53:TRP:CD1	2.55	0.90
23:T:47:PRO:HB3	23:T:53:TRP:CD1	2.06	0.90
33:d:21:CYS:HB2	33:d:30:LEU:CD1	2.01	0.90
38:i:51:CYS:SG	38:i:55:ASN:O	2.30	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:g:8:LEU:HD13	36:g:269:ILE:HD12	1.50	0.89
6:C:43:VAL:HG13	6:C:44:THR:H	1.35	0.89
28:Y:29:HIS:NE2	28:Y:34:ASN:O	2.04	0.89
40:k:322:ASP:OD2	40:k:404:PRO:HB3	1.72	0.89
36:g:258:TRP:CE2	36:g:278:ILE:HD13	2.08	0.89
2:2:1392:G:P	36:g:292:GLN:NE2	2.44	0.89
11:H:162:ILE:HG22	11:H:166:LEU:HD21	1.52	0.89
15:L:87:ARG:CZ	15:L:104:HIS:HB2	2.02	0.89
12:I:154:GLU:HG2	12:I:155:HIS:N	1.84	0.89
14:K:83:PRO:O	14:K:86:ILE:HD13	1.73	0.89
36:g:285:PHE:HE1	36:g:318:ARG:CZ	1.86	0.89
16:M:82:VAL:HG21	16:M:88:LEU:HD11	1.54	0.88
12:I:40:THR:O	12:I:59:ARG:HB3	1.71	0.88
31:b:2:VAL:HG23	31:b:3:LEU:H	1.38	0.88
39:j:38:GLU:N	39:j:38:GLU:OE2	2.05	0.88
44:p:294:VAL:HG13	44:p:303:PHE:CE1	2.07	0.88
22:S:11:PHE:CE2	22:S:57:ARG:CZ	2.57	0.88
27:X:63:GLN:O	27:X:65:ASN:N	2.07	0.88
36:g:179:MET:HG2	36:g:205:TYR:HD1	1.36	0.88
42:m:73:GLU:OE1	42:m:73:GLU:N	2.05	0.88
22:S:12:GLN:H	22:S:59:GLY:HA3	1.38	0.88
32:c:34:GLU:OE1	32:c:34:GLU:N	2.07	0.87
36:g:47:ARG:NE	36:g:59:VAL:HG11	1.89	0.87
21:R:23:LYS:HE3	36:g:205:TYR:HH	1.37	0.87
5:B:117:TRP:CE3	5:B:153:THR:HG22	2.05	0.87
33:d:23:ILE:HD13	33:d:46:LYS:HZ2	1.28	0.87
40:k:136:ILE:HD12	40:k:137:THR:H	1.37	0.87
5:B:128:LYS:CE	5:B:132:ASP:HA	2.01	0.87
14:K:61:TRP:O	14:K:62:GLN:HG2	1.74	0.87
26:W:30:SER:HG	26:W:61:ILE:HD11	1.36	0.87
39:j:225:ALA:HB3	39:j:226:PRO:HD3	1.54	0.87
40:k:125:THR:HG21	40:k:137:THR:HG22	1.54	0.87
3:A:81:TYR:CD2	3:A:167:LYS:CD	2.58	0.87
7:D:71:LEU:HD11	14:K:89:ALA:HB1	1.55	0.87
10:G:68:LEU:O	10:G:101:ILE:HD11	1.75	0.87
25:V:10:GLU:HG3	25:V:12:TYR:O	1.74	0.87
39:j:190:VAL:O	39:j:226:PRO:O	1.93	0.87
36:g:258:TRP:CE2	36:g:278:ILE:CD1	2.58	0.86
3:A:88:LYS:CB	3:A:202:TYR:HD1	1.88	0.86
34:e:10:ARG:CZ	34:e:13:LYS:HG2	2.05	0.86
44:p:343:TYR:OH	44:p:346:LYS:CD	2.22	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:p:403:LEU:O	44:p:420:ALA:O	1.92	0.86
28:Y:29:HIS:HD2	28:Y:34:ASN:O	1.13	0.86
9:F:127:THR:O	9:F:129:GLN:NE2	2.08	0.86
22:S:12:GLN:H	22:S:59:GLY:CA	1.88	0.86
26:W:76:SER:HB3	26:W:77:PRO:HD3	1.57	0.85
2:2:1228:G:N7	35:f:102:VAL:HG12	1.90	0.85
14:K:54:PHE:CZ	14:K:71:GLU:OE2	2.29	0.85
20:Q:113:ASP:HA	20:Q:116:LEU:HD12	1.57	0.85
30:a:10:ARG:HA	30:a:34:LYS:HE2	1.56	0.85
30:a:37:LYS:O	30:a:38:ARG:CZ	2.24	0.85
36:g:172:ILE:HG21	36:g:174:PHE:CE2	2.10	0.85
23:T:34:VAL:HG13	23:T:54:PHE:CD2	2.11	0.85
33:d:19:ARG:HB2	33:d:32:ARG:HH21	1.42	0.85
35:f:107:LYS:NZ	35:f:116:LYS:C	2.34	0.85
7:D:219:GLU:HG2	7:D:220:PRO:HD3	1.54	0.85
36:g:8:LEU:CD1	36:g:269:ILE:HD13	2.07	0.85
39:j:74:LEU:CD2	39:j:89:ARG:NH1	2.39	0.85
35:f:111:GLU:N	35:f:111:GLU:OE2	2.09	0.85
40:k:164:PHE:N	40:k:177:PRO:O	2.08	0.85
25:V:10:GLU:O	25:V:11:LEU:HG	1.76	0.84
36:g:6:ILE:CG2	36:g:322:VAL:CG1	2.55	0.84
28:Y:5:ILE:CD1	28:Y:32:ARG:HH11	1.90	0.84
35:f:107:LYS:NZ	35:f:116:LYS:O	2.10	0.84
36:g:154:LYS:CD	36:g:208:VAL:HG23	2.06	0.84
8:E:11:ARG:HE	8:E:25:GLY:CA	1.73	0.84
22:S:11:PHE:CD2	22:S:57:ARG:NH1	2.45	0.84
25:V:40:ASP:HB3	25:V:44:ARG:O	1.77	0.84
36:g:29:ALA:CB	36:g:77:ASP:HA	2.08	0.84
36:g:154:LYS:HZ3	36:g:208:VAL:CG2	1.91	0.84
3:A:88:LYS:HB3	3:A:202:TYR:CE1	2.11	0.84
44:p:294:VAL:HG13	44:p:303:PHE:HE1	1.40	0.84
6:C:147:GLY:C	6:C:156:PRO:CB	2.51	0.84
36:g:6:ILE:HG23	36:g:322:VAL:CG1	2.07	0.84
22:S:11:PHE:HB2	22:S:60:GLU:N	1.91	0.84
33:d:21:CYS:SG	33:d:23:ILE:HG22	2.17	0.84
24:U:22:ILE:HG22	24:U:93:LEU:O	1.78	0.83
25:V:10:GLU:O	25:V:11:LEU:CG	2.26	0.83
25:V:10:GLU:O	25:V:11:LEU:HD12	1.78	0.83
36:g:126:ALA:HB2	36:g:155:VAL:CG1	2.07	0.83
36:g:154:LYS:HE3	36:g:207:ASN:O	1.78	0.83
36:g:156:ARG:HE	36:g:210:GLN:HE22	1.23	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:77:SER:HB2	3:A:86:VAL:HG21	1.60	0.83
22:S:26:ILE:HG22	22:S:30:TYR:HB2	1.60	0.83
28:Y:29:HIS:CE1	28:Y:32:ARG:O	2.31	0.83
39:j:74:LEU:HD21	39:j:89:ARG:NH1	1.93	0.83
11:H:73:VAL:O	11:H:75:ILE:N	2.11	0.83
33:d:21:CYS:HB3	33:d:24:SER:O	1.78	0.83
33:d:31:ILE:HG12	33:d:38:ILE:H	1.44	0.83
36:g:154:LYS:CE	36:g:208:VAL:HB	2.07	0.83
8:E:241:GLY:O	8:E:244:ILE:HG22	1.79	0.83
21:R:23:LYS:HE2	36:g:205:TYR:OH	1.76	0.83
36:g:74:VAL:CG1	36:g:78:GLY:HA2	2.08	0.83
36:g:285:PHE:HE1	36:g:318:ARG:NH2	1.77	0.83
11:H:31:SER:HA	11:H:35:LYS:HB2	1.61	0.82
30:a:12:LYS:HA	30:a:15:ARG:NH2	1.92	0.82
36:g:204:ASN:HD22	36:g:224:ASP:CB	1.91	0.82
42:m:93:ILE:O	42:m:98:LEU:HD23	1.79	0.82
13:J:35:GLY:HA3	13:J:122:VAL:HG11	1.58	0.82
36:g:258:TRP:CD2	36:g:278:ILE:HD13	2.14	0.82
30:a:22:ARG:HE	30:a:27:SER:HB3	1.45	0.82
35:f:107:LYS:HZ3	35:f:116:LYS:H	1.28	0.82
36:g:6:ILE:CG2	36:g:322:VAL:HG13	2.09	0.82
22:S:29:VAL:O	22:S:33:THR:HG23	1.79	0.82
38:i:49:ALA:HB3	38:i:57:ARG:O	1.80	0.82
23:T:47:PRO:HB3	23:T:53:TRP:CE2	2.15	0.82
26:W:30:SER:CB	26:W:61:ILE:HG13	2.10	0.81
36:g:258:TRP:CD1	36:g:278:ILE:HD11	2.15	0.81
33:d:22:ARG:NH2	33:d:35:GLY:O	2.13	0.81
36:g:172:ILE:CG2	36:g:174:PHE:CE2	2.62	0.81
20:Q:140:LYS:HD2	20:Q:142:TYR:CE2	2.15	0.81
27:X:20:ARG:O	27:X:24:TRP:HD1	1.63	0.81
36:g:126:ALA:HB1	36:g:152:VAL:CG1	2.10	0.81
3:A:90:ALA:O	3:A:93:THR:O	1.98	0.81
39:j:40:ASP:OD1	39:j:41:ASN:N	2.11	0.81
14:K:64:TYR:HB3	14:K:66:TYR:HE2	1.45	0.81
35:f:98:VAL:CG1	35:f:100:LEU:CD2	2.58	0.81
44:p:314:ILE:HD12	44:p:323:MET:HB2	1.62	0.81
8:E:77:ARG:HG3	8:E:77:ARG:HH11	1.46	0.81
39:j:5:HIS:HB2	39:j:41:ASN:ND2	1.96	0.81
40:k:128:PHE:CD1	40:k:132:LEU:HD12	2.13	0.81
3:A:88:LYS:CG	3:A:202:TYR:HD1	1.94	0.81
44:p:620:ARG:HG3	44:p:621:TYR:CD2	2.16	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:10:ARG:HA	30:a:34:LYS:CE	2.08	0.81
2:2:1228:G:N7	35:f:102:VAL:CG1	2.44	0.80
6:C:148:TYR:CD2	6:C:156:PRO:HB3	2.16	0.80
40:k:127:ARG:NH2	51:k:602:GCP:O2B	2.13	0.80
13:J:170:GLY:O	13:J:174:ARG:HD3	1.81	0.80
6:C:147:GLY:O	6:C:156:PRO:CB	2.26	0.80
21:R:29:GLN:HB3	36:g:86:TRP:CH2	2.16	0.80
38:i:51:CYS:HB2	38:i:55:ASN:C	2.05	0.80
10:G:32:ILE:HD11	10:G:63:MET:SD	2.21	0.80
36:g:289:THR:OG1	36:g:292:GLN:HG2	1.81	0.80
3:A:88:LYS:CD	3:A:202:TYR:HD1	1.95	0.80
3:A:168:HIS:HA	3:A:203:PHE:HE2	1.40	0.80
9:F:44:LEU:CD2	9:F:49:SER:HA	2.11	0.80
9:F:45:PHE:CZ	9:F:72:VAL:HA	2.16	0.80
14:K:21:LEU:HD22	14:K:32:HIS:CE1	2.17	0.80
22:S:11:PHE:HA	22:S:59:GLY:C	2.06	0.80
26:W:6:VAL:HG13	26:W:29:PRO:HG2	1.63	0.80
36:g:277:LEU:HD21	36:g:280:GLU:HG3	1.64	0.80
13:J:113:VAL:O	13:J:117:GLY:HA3	1.80	0.80
39:j:28:ALA:N	39:j:31:GLY:O	2.15	0.80
40:k:127:ARG:O	40:k:133:GLU:CG	2.29	0.80
3:A:81:TYR:HD2	3:A:167:LYS:CD	1.93	0.80
14:K:54:PHE:CE2	14:K:71:GLU:OE2	2.35	0.80
27:X:92:CYS:CB	27:X:95:PHE:CD1	2.65	0.80
36:g:260:THR:HG21	36:g:301:TRP:CZ2	2.17	0.79
40:k:381:PHE:CE1	40:k:382:ALA:O	2.36	0.79
45:q:174:VAL:O	45:q:178:VAL:HG13	1.83	0.79
12:I:67:TRP:HD1	12:I:70:GLU:H	1.26	0.79
23:T:47:PRO:HB3	23:T:53:TRP:NE1	1.97	0.79
30:a:36:ILE:HD11	30:a:75:ILE:HA	1.64	0.79
36:g:258:TRP:CD2	36:g:278:ILE:CD1	2.65	0.79
22:S:11:PHE:HE2	22:S:57:ARG:HH12	1.30	0.79
35:f:98:VAL:C	35:f:99:LYS:HD2	2.07	0.79
36:g:107:HIS:HA	36:g:133:ARG:NH2	1.94	0.79
3:A:63:ILE:HD11	3:A:158:VAL:HG21	1.64	0.79
8:E:21:ASP:OD2	8:E:24:SER:HB2	1.83	0.79
19:P:126:VAL:HB	19:P:128:HIS:CD2	2.18	0.79
22:S:12:GLN:N	22:S:59:GLY:HA3	1.97	0.79
36:g:260:THR:CG2	36:g:301:TRP:HZ2	1.95	0.79
30:a:36:ILE:O	30:a:73:TYR:HD1	1.65	0.79
27:X:21:ASN:HA	27:X:24:TRP:HD1	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:f:105:TYR:CE2	35:f:106:TYR:CZ	2.72	0.78
36:g:8:LEU:CD1	36:g:269:ILE:HD12	2.12	0.78
36:g:156:ARG:NE	36:g:210:GLN:HE22	1.80	0.78
3:A:167:LYS:O	3:A:170:ILE:HD13	1.84	0.78
40:k:127:ARG:O	40:k:133:GLU:HG2	1.84	0.78
44:p:324:ALA:HB3	44:p:365:PHE:CE1	2.18	0.78
38:i:36:ALA:N	38:i:52:PHE:HE2	1.80	0.78
44:p:700:ARG:CB	44:p:711:LYS:CB	2.62	0.78
40:k:136:ILE:HD12	40:k:137:THR:C	2.08	0.78
45:q:510:THR:CG2	45:q:514:LYS:HD2	2.14	0.78
27:X:20:ARG:C	27:X:24:TRP:CD1	2.61	0.78
30:a:36:ILE:HD12	30:a:78:ALA:CB	2.08	0.78
29:Z:84:GLU:OE2	29:Z:89:ILE:HD12	1.84	0.78
36:g:260:THR:CG2	36:g:301:TRP:CZ2	2.66	0.78
28:Y:5:ILE:HD13	28:Y:32:ARG:HH11	1.48	0.78
41:l:139:PHE:O	41:l:142:LEU:HD13	1.84	0.78
39:j:57:ARG:N	39:j:57:ARG:HH11	1.82	0.77
21:R:75:GLU:OE1	21:R:75:GLU:N	2.18	0.77
33:d:23:ILE:HD13	33:d:46:LYS:HZ1	1.48	0.77
8:E:11:ARG:HE	8:E:25:GLY:HA3	0.95	0.77
39:j:38:GLU:OE1	39:j:102:TYR:HD1	1.60	0.77
10:G:32:ILE:HA	10:G:52:ILE:HG23	1.67	0.77
2:2:1099:G:O2'	26:W:76:SER:N	2.16	0.77
9:F:45:PHE:HE1	9:F:117:LYS:HZ3	1.31	0.77
29:Z:57:TYR:CD2	29:Z:59:TYR:O	2.38	0.77
40:k:136:ILE:CD1	40:k:137:THR:O	2.32	0.77
36:g:208:VAL:HG11	36:g:249:ALA:HA	1.67	0.77
14:K:21:LEU:CD2	14:K:32:HIS:CE1	2.68	0.77
36:g:179:MET:CG	36:g:205:TYR:HD1	1.97	0.77
27:X:92:CYS:C	27:X:95:PHE:HD1	1.93	0.76
36:g:260:THR:HG22	36:g:269:ILE:HG12	1.65	0.76
44:p:316:ASP:OD1	44:p:323:MET:CE	2.33	0.76
29:Z:68:ARG:HH22	29:Z:70:LYS:HG3	1.49	0.76
5:B:117:TRP:HB3	5:B:153:THR:HG22	1.67	0.76
12:I:154:GLU:CG	12:I:155:HIS:H	1.97	0.76
44:p:179:ASP:O	44:p:181:PRO:HD3	1.84	0.76
22:S:29:VAL:CG2	22:S:44:ASN:HA	2.16	0.76
36:g:8:LEU:HD11	36:g:269:ILE:HD13	1.66	0.76
3:A:63:ILE:CD1	3:A:158:VAL:HG21	2.15	0.76
30:a:62:TYR:CE2	30:a:65:PRO:HD3	2.20	0.76
39:j:119:PHE:CB	39:j:121:ILE:HD11	2.14	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:59:TYR:CE1	30:a:62:TYR:CD1	2.74	0.76
39:j:94:ASP:OD1	39:j:98:CYS:HB2	1.85	0.76
40:k:208:ALA:HB3	40:k:239:MET:HG3	1.66	0.76
40:k:289:TYR:O	40:k:291:ILE:HG13	1.85	0.76
21:R:21:TYR:N	21:R:22:PRO:HD2	1.99	0.76
23:T:47:PRO:HB2	23:T:53:TRP:CD1	2.19	0.76
28:Y:35:VAL:HG21	28:Y:40:LEU:HD11	1.67	0.76
35:f:98:VAL:CG1	35:f:100:LEU:HD21	2.16	0.76
20:Q:140:LYS:HD2	20:Q:142:TYR:CZ	2.20	0.76
45:q:509:TYR:CE2	45:q:514:LYS:NZ	2.54	0.76
36:g:179:MET:HG2	36:g:205:TYR:CD1	2.20	0.76
40:k:125:THR:CG2	40:k:137:THR:HG21	2.16	0.76
2:2:1101:G:OP1	26:W:76:SER:OG	2.03	0.75
9:F:118:HIS:O	9:F:122:ILE:HG12	1.86	0.75
40:k:238:ILE:HD13	40:k:513:GLY:O	1.86	0.75
33:d:31:ILE:O	33:d:37:ASN:HA	1.86	0.75
40:k:238:ILE:CG2	40:k:514:TRP:CB	2.61	0.75
38:i:36:ALA:HA	38:i:52:PHE:CE2	2.22	0.75
14:K:55:VAL:HG22	14:K:68:LEU:CD2	2.16	0.75
14:K:83:PRO:O	14:K:86:ILE:CD1	2.34	0.75
36:g:124:ILE:HD13	36:g:174:PHE:CE1	2.21	0.75
35:f:105:TYR:CE2	35:f:106:TYR:CE2	2.74	0.75
2:2:71:A:C3'	2:2:72:A:H5''	2.06	0.75
8:E:181:VAL:HG12	8:E:193:GLY:O	1.86	0.75
36:g:82:VAL:HG11	36:g:114:VAL:CG2	2.17	0.75
44:p:281:GLU:HB3	44:p:317:ILE:HD13	1.67	0.75
28:Y:2:SER:C	28:Y:31:ASN:OD1	2.30	0.75
30:a:59:TYR:CE1	30:a:62:TYR:HB2	2.20	0.75
36:g:258:TRP:NE1	36:g:278:ILE:HD11	2.01	0.75
8:E:105:VAL:O	8:E:245:LYS:HE3	1.87	0.74
35:f:107:LYS:NZ	35:f:116:LYS:H	1.82	0.74
36:g:43:LEU:CD2	36:g:72:VAL:HG21	2.16	0.74
38:i:35:TYR:C	38:i:52:PHE:CE2	2.65	0.74
17:N:114:ARG:O	17:N:118:ILE:HG12	1.87	0.74
39:j:29:GLU:OE2	39:j:30:MET:HG3	1.86	0.74
44:p:324:ALA:HB3	44:p:365:PHE:HE1	1.52	0.74
7:D:200:LYS:HE2	7:D:201:ALA:N	2.01	0.74
36:g:78:GLY:C	36:g:95:LEU:HD12	2.12	0.74
40:k:474:ARG:O	40:k:485:LEU:HD23	1.87	0.74
44:p:314:ILE:HD13	44:p:323:MET:HB2	1.67	0.74
5:B:210:VAL:O	5:B:211:HIS:CD2	2.41	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:g:81:ALA:HB2	36:g:95:LEU:CD2	2.17	0.74
36:g:154:LYS:NZ	36:g:208:VAL:CG2	2.48	0.74
44:p:79:ILE:HD12	44:p:131:CYS:SG	2.28	0.74
8:E:73:ASP:C	8:E:164:LEU:HD21	2.13	0.74
14:K:87:PHE:CD2	14:K:91:TYR:CD2	2.76	0.74
39:j:74:LEU:HD21	39:j:89:ARG:HH11	1.51	0.74
24:U:106:ILE:HD12	24:U:107:THR:N	2.03	0.74
11:H:85:PHE:HD2	11:H:88:ARG:HE	1.33	0.74
40:k:136:ILE:CA	51:k:602:GCP:H3B1	2.17	0.74
5:B:25:THR:O	5:B:27:LYS:N	2.21	0.73
9:F:128:ASP:C	9:F:129:GLN:HE21	1.95	0.73
22:S:29:VAL:HG21	22:S:44:ASN:HA	1.69	0.73
8:E:71:LYS:HE2	8:E:76:VAL:CG2	2.12	0.73
39:j:48:LEU:HD22	39:j:56:ILE:HD11	1.68	0.73
21:R:29:GLN:HB3	36:g:86:TRP:HZ3	1.47	0.73
27:X:97:ASP:O	27:X:100:ASP:HB2	1.87	0.73
40:k:130:ASP:OD1	40:k:134:ARG:HD2	1.89	0.73
36:g:82:VAL:HG12	36:g:114:VAL:HG21	1.68	0.73
6:C:43:VAL:HG22	6:C:44:THR:HG23	1.69	0.73
20:Q:93:HIS:HB3	20:Q:102:LYS:HG2	1.70	0.73
35:f:105:TYR:CZ	35:f:106:TYR:CE2	2.75	0.73
33:d:34:TYR:HB2	33:d:36:LEU:CD1	2.15	0.73
36:g:143:TYR:CD2	36:g:193:TYR:CZ	2.77	0.73
2:2:1659:U:H2'	2:2:1660:G:H8	1.54	0.73
2:2:1476:G:H1'	23:T:53:TRP:HZ3	1.52	0.73
11:H:162:ILE:O	11:H:166:LEU:HG	1.87	0.73
22:S:48:LYS:NZ	23:T:48:GLN:O	2.22	0.73
36:g:62:TYR:CE1	36:g:98:GLY:HA2	2.24	0.73
14:K:55:VAL:HG22	14:K:68:LEU:HD23	1.70	0.73
36:g:231:ASN:CG	36:g:234:HIS:HD2	1.94	0.72
43:o:702:UNK:O	43:o:705:UNK:N	2.22	0.72
45:q:255:PHE:HD1	45:q:259:GLN:OE1	1.72	0.72
10:G:149:LYS:HG2	10:G:150:GLU:H	1.54	0.72
30:a:64:LEU:C	30:a:64:LEU:HD23	2.13	0.72
18:O:111:ARG:HD3	30:a:58:VAL:HG22	1.69	0.72
36:g:133:ARG:HG2	36:g:144:VAL:HG22	1.71	0.72
32:c:13:ILE:C	32:c:14:LYS:HD2	2.15	0.72
36:g:74:VAL:HG11	36:g:78:GLY:HA2	1.71	0.72
35:f:97:LYS:C	35:f:99:LYS:HE3	2.13	0.72
40:k:136:ILE:CD1	40:k:137:THR:C	2.62	0.72
29:Z:57:TYR:CE2	29:Z:59:TYR:O	2.43	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:g:112:LEU:HD11	36:g:128:ARG:HG3	1.69	0.72
36:g:124:ILE:CD1	36:g:174:PHE:CD1	2.70	0.72
38:i:36:ALA:CA	38:i:52:PHE:HE2	2.02	0.72
2:2:1086:A:H2'	2:2:1087:A:C8	2.25	0.72
18:O:89:THR:O	18:O:128:LYS:HE3	1.90	0.72
39:j:28:ALA:CB	39:j:31:GLY:C	2.60	0.72
3:A:168:HIS:CA	3:A:203:PHE:CE2	2.68	0.72
30:a:36:ILE:O	30:a:73:TYR:CD1	2.43	0.72
35:f:98:VAL:HG12	35:f:100:LEU:HD21	1.68	0.72
16:M:67:LEU:HD21	35:f:106:TYR:CE1	2.24	0.71
38:i:85:GLN:OE1	38:i:87:ASP:HB2	1.90	0.71
40:k:277:GLY:O	40:k:278:ALA:HB2	1.89	0.71
22:S:29:VAL:HG13	22:S:43:ALA:HB3	1.72	0.71
32:c:33:LEU:HD23	32:c:33:LEU:H	1.54	0.71
40:k:238:ILE:HG12	40:k:514:TRP:HB3	1.72	0.71
39:j:38:GLU:OE1	39:j:102:TYR:CE1	2.42	0.71
8:E:71:LYS:HG2	8:E:76:VAL:HA	1.71	0.71
11:H:98:ILE:HG12	11:H:121:VAL:CG1	2.15	0.71
30:a:62:TYR:CE2	30:a:64:LEU:HA	2.25	0.71
36:g:29:ALA:HB2	36:g:77:ASP:HA	1.71	0.71
11:H:160:GLN:HA	11:H:163:ASP:OD2	1.89	0.71
20:Q:137:ARG:HH11	20:Q:137:ARG:HB2	1.55	0.71
27:X:21:ASN:HA	27:X:24:TRP:CD1	2.24	0.71
27:X:21:ASN:CA	27:X:24:TRP:HD1	2.03	0.71
14:K:92:LEU:HD23	14:K:93:ALA:N	2.06	0.71
21:R:113:LEU:O	21:R:115:LEU:HG	1.91	0.71
14:K:87:PHE:HD2	14:K:91:TYR:CD2	2.09	0.71
39:j:121:ILE:HD13	39:j:121:ILE:N	2.05	0.71
3:A:81:TYR:CD2	3:A:167:LYS:HD2	2.26	0.71
14:K:21:LEU:CD2	14:K:32:HIS:HE1	2.04	0.71
30:a:62:TYR:HE2	30:a:64:LEU:HA	1.56	0.71
40:k:238:ILE:CG1	40:k:514:TRP:HB3	2.21	0.71
3:A:41:ARG:HG2	3:A:42:PRO:HD2	1.73	0.71
38:i:36:ALA:N	38:i:52:PHE:CE2	2.59	0.71
5:B:117:TRP:HE3	5:B:153:THR:HG21	1.53	0.70
16:M:120:ASP:OD2	16:M:124:ARG:HD2	1.90	0.70
29:Z:64:VAL:O	29:Z:68:ARG:HG3	1.91	0.70
44:p:620:ARG:HG3	44:p:621:TYR:CE2	2.26	0.70
16:M:33:GLY:C	16:M:34:LEU:HD12	2.16	0.70
28:Y:29:HIS:HE1	28:Y:33:ALA:CA	1.82	0.70
36:g:228:TYR:CZ	36:g:240:ASN:ND2	2.60	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:I:41:LYS:HD3	12:I:43:ILE:CD1	2.22	0.70
12:I:67:TRP:CD1	12:I:70:GLU:H	2.07	0.70
24:U:27:THR:CG2	24:U:88:LYS:HG2	2.21	0.70
25:V:11:LEU:HD12	25:V:11:LEU:C	2.16	0.70
36:g:174:PHE:HD2	36:g:188:LEU:HG	1.56	0.70
38:i:36:ALA:CA	38:i:52:PHE:CE2	2.75	0.70
40:k:125:THR:CG2	40:k:137:THR:CG2	2.64	0.70
24:U:27:THR:HG22	24:U:88:LYS:HG2	1.73	0.70
25:V:10:GLU:C	25:V:11:LEU:HG	2.17	0.70
9:F:153:GLY:CA	9:F:158:ARG:HH11	2.04	0.70
40:k:136:ILE:CD1	40:k:137:THR:H	1.93	0.70
44:p:359:HIS:HB3	44:p:365:PHE:HD2	1.56	0.70
29:Z:84:GLU:CD	29:Z:89:ILE:HD12	2.16	0.70
30:a:37:LYS:O	30:a:38:ARG:NH2	2.25	0.70
42:m:93:ILE:O	42:m:98:LEU:CD2	2.40	0.70
14:K:16:PHE:O	14:K:88:PRO:CB	2.40	0.69
14:K:87:PHE:HA	14:K:91:TYR:CD1	2.26	0.69
39:j:14:PRO:HG3	39:j:40:ASP:CB	2.22	0.69
14:K:54:PHE:CE2	14:K:75:TYR:CD1	2.79	0.69
2:2:385:G:H2'	2:2:386:A:H8	1.56	0.69
21:R:110:VAL:O	21:R:114:GLY:N	2.25	0.69
2:2:1659:U:H2'	2:2:1660:G:C8	2.27	0.69
1:1:27:C:H2'	1:1:28:A:C8	2.27	0.69
23:T:47:PRO:HB3	23:T:53:TRP:CG	2.26	0.69
40:k:98:GLN:CG	40:k:391:VAL:HB	2.22	0.69
40:k:238:ILE:HG12	40:k:514:TRP:CE3	2.27	0.69
8:E:71:LYS:NZ	8:E:76:VAL:HG22	2.07	0.69
19:P:126:VAL:HB	19:P:128:HIS:HD2	1.57	0.69
2:2:1020:C:O5'	45:q:115:ALA:HB2	1.93	0.69
3:A:92:HIS:CE1	3:A:202:TYR:HH	2.11	0.69
6:C:148:TYR:OH	6:C:154:GLY:C	2.36	0.69
13:J:35:GLY:CA	13:J:122:VAL:HG11	2.22	0.69
39:j:225:ALA:CB	39:j:226:PRO:HD3	2.23	0.69
40:k:381:PHE:CD1	40:k:382:ALA:O	2.46	0.69
2:2:1021:C:H4'	2:2:1124:A:H61	1.58	0.69
27:X:92:CYS:N	27:X:95:PHE:HE1	1.76	0.69
30:a:62:TYR:HE2	30:a:65:PRO:HD3	1.58	0.69
39:j:14:PRO:HG3	39:j:40:ASP:HB3	1.75	0.69
11:H:73:VAL:O	11:H:75:ILE:HG12	1.92	0.69
20:Q:94:GLN:HE22	36:g:63:LYS:HE3	1.55	0.69
36:g:25:SER:OG	36:g:35:VAL:HB	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:g:43:LEU:HD21	36:g:72:VAL:CG2	2.22	0.68
44:p:390:LEU:HD22	44:p:477:ASP:O	1.93	0.68
26:W:30:SER:OG	26:W:61:ILE:CG1	2.41	0.68
36:g:126:ALA:HB1	36:g:152:VAL:HG12	1.74	0.68
36:g:258:TRP:CE2	36:g:278:ILE:HD11	2.27	0.68
11:H:8:ILE:O	11:H:42:GLN:HG2	1.93	0.68
2:2:707:A:H61	2:2:730:G:H22	1.41	0.68
13:J:162:SER:HB2	13:J:163:PRO:HD2	1.75	0.68
36:g:228:TYR:CE1	36:g:240:ASN:ND2	2.60	0.68
39:j:17:ASP:HA	39:j:73:VAL:O	1.94	0.68
13:J:35:GLY:HA3	13:J:122:VAL:HG12	1.74	0.68
21:R:21:TYR:N	21:R:22:PRO:CD	2.56	0.68
22:S:18:LEU:CD2	22:S:19:ASN:H	2.06	0.68
35:f:119:LYS:HE3	35:f:119:LYS:CA	2.23	0.68
40:k:208:ALA:CB	40:k:239:MET:HG3	2.23	0.68
36:g:283:PRO:HB2	36:g:285:PHE:CZ	2.29	0.68
29:Z:39:ALA:O	29:Z:40:VAL:CG2	2.42	0.68
3:A:41:ARG:HD2	3:A:43:ASP:OD2	1.92	0.68
8:E:11:ARG:HD2	8:E:25:GLY:CA	2.17	0.68
36:g:231:ASN:HD21	36:g:234:HIS:HD2	0.69	0.68
36:g:260:THR:HG23	36:g:301:TRP:HZ2	1.57	0.68
36:g:277:LEU:HD21	36:g:280:GLU:CG	2.24	0.68
8:E:76:VAL:O	8:E:77:ARG:NE	2.26	0.68
36:g:112:LEU:HD12	36:g:152:VAL:O	1.92	0.68
22:S:11:PHE:CD2	22:S:57:ARG:HD3	2.29	0.67
39:j:74:LEU:HD11	39:j:89:ARG:CZ	2.24	0.67
14:K:21:LEU:HD23	14:K:32:HIS:HE1	1.58	0.67
14:K:88:PRO:HD3	14:K:91:TYR:HE1	1.59	0.67
22:S:18:LEU:HD23	22:S:19:ASN:H	1.59	0.67
22:S:6:GLN:OE1	22:S:7:GLU:N	2.27	0.67
29:Z:68:ARG:CZ	29:Z:70:LYS:HG3	2.25	0.67
36:g:174:PHE:CD2	36:g:188:LEU:HG	2.29	0.67
36:g:265:SER:O	36:g:282:LYS:HE2	1.94	0.67
40:k:98:GLN:HG2	40:k:391:VAL:HB	1.76	0.67
30:a:36:ILE:HD13	30:a:78:ALA:CB	2.23	0.67
2:2:1476:G:H1'	23:T:53:TRP:CZ3	2.28	0.67
27:X:109:ARG:HB3	27:X:112:LYS:HB2	1.77	0.67
3:A:70:PRO:HB3	3:A:94:GLY:HA3	1.77	0.67
26:W:23:ARG:HG3	31:b:4:VAL:HG22	1.76	0.67
29:Z:84:GLU:HG2	29:Z:89:ILE:HB	1.75	0.67
14:K:21:LEU:HD21	14:K:35:ILE:HD11	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:S:11:PHE:HB2	22:S:59:GLY:C	2.19	0.66
2:2:1755:G:OP2	38:i:43:GLY:O	2.13	0.66
11:H:8:ILE:CD1	11:H:21:ALA:HB1	2.24	0.66
30:a:36:ILE:CB	30:a:73:TYR:HB2	2.19	0.66
36:g:174:PHE:CD2	36:g:188:LEU:CD1	2.78	0.66
36:g:187:SER:OG	36:g:192:SER:OG	2.13	0.66
36:g:269:ILE:HG22	36:g:278:ILE:HD12	1.77	0.66
37:h:6:ARG:HA	37:h:9:ARG:HD3	1.77	0.66
2:2:1290:G:H22	2:2:1323:G:H22	1.44	0.66
35:f:119:LYS:HA	35:f:119:LYS:CE	2.21	0.66
43:o:718:UNK:HA	44:p:194:MET:CB	2.25	0.66
30:a:12:LYS:O	30:a:12:LYS:HD3	1.95	0.66
36:g:47:ARG:CG	36:g:59:VAL:HG11	2.25	0.66
36:g:47:ARG:HG3	36:g:59:VAL:HG11	1.78	0.66
40:k:136:ILE:HD12	40:k:136:ILE:C	2.18	0.66
5:B:24:PHE:CE2	5:B:27:LYS:NZ	2.64	0.66
15:L:87:ARG:HH22	15:L:104:HIS:HB2	1.55	0.66
10:G:14:LYS:NZ	10:G:122:GLU:HB2	2.11	0.66
12:I:36:THR:O	12:I:96:LEU:N	2.28	0.66
28:Y:2:SER:O	28:Y:31:ASN:OD1	2.14	0.66
30:a:59:TYR:HE1	30:a:62:TYR:CB	2.07	0.66
36:g:6:ILE:HG23	36:g:322:VAL:HG12	1.77	0.66
28:Y:5:ILE:HD12	28:Y:5:ILE:N	2.11	0.66
35:f:100:LEU:HD22	35:f:100:LEU:N	2.10	0.66
36:g:172:ILE:HG21	36:g:174:PHE:CZ	2.31	0.66
1:1:64:RIA:N3	1:1:64:RIA:H1'	2.10	0.65
3:A:81:TYR:HB3	3:A:167:LYS:HG3	1.77	0.65
29:Z:68:ARG:HH12	29:Z:70:LYS:CE	2.09	0.65
10:G:152:ASP:OD2	10:G:154:ARG:HB2	1.96	0.65
12:I:84:HIS:HB3	12:I:91:VAL:HG22	1.77	0.65
36:g:272:LEU:HD12	36:g:272:LEU:N	2.10	0.65
11:H:73:VAL:HG13	11:H:74:GLN:H	1.62	0.65
19:P:127:ARG:NE	19:P:127:ARG:HA	2.10	0.65
36:g:208:VAL:HG11	36:g:249:ALA:CA	2.27	0.65
39:j:57:ARG:HD2	39:j:57:ARG:N	2.08	0.65
44:p:210:THR:HB	44:p:231:TRP:CE3	2.30	0.65
10:G:31:ARG:HD2	10:G:68:LEU:HD12	1.79	0.65
10:G:142:ARG:NE	10:G:149:LYS:HA	2.12	0.65
24:U:21:LYS:HD2	24:U:21:LYS:N	2.11	0.65
36:g:74:VAL:HG12	36:g:75:SER:O	1.96	0.65
36:g:285:PHE:CE1	36:g:318:ARG:NH2	2.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:p:316:ASP:CG	44:p:323:MET:HE2	2.21	0.65
16:M:97:ILE:HG12	16:M:104:ARG:HH21	1.59	0.65
14:K:54:PHE:CZ	14:K:75:TYR:CD1	2.85	0.65
40:k:135:ASN:O	40:k:136:ILE:HG13	1.97	0.65
3:A:73:VAL:HG13	3:A:120:LEU:HD12	1.79	0.65
40:k:495:ILE:HG22	40:k:496:ASN:H	1.61	0.65
45:q:510:THR:HA	45:q:514:LYS:HD2	1.79	0.65
9:F:153:GLY:CA	9:F:156:ALA:O	2.41	0.65
11:H:45:SER:C	11:H:46:ILE:HD12	2.22	0.65
40:k:127:ARG:CB	40:k:133:GLU:HA	2.27	0.65
40:k:322:ASP:CG	40:k:404:PRO:HB3	2.21	0.65
45:q:381:MET:HG3	45:q:607:PRO:HD3	1.77	0.65
2:2:1443:G:C2	35:f:90:LYS:O	2.49	0.65
11:H:98:ILE:CG2	11:H:118:LEU:HD23	2.27	0.65
24:U:49:LYS:N	24:U:49:LYS:HD2	2.11	0.65
26:W:6:VAL:CG1	26:W:29:PRO:HG2	2.27	0.65
28:Y:5:ILE:HD13	28:Y:32:ARG:NH1	2.12	0.65
39:j:5:HIS:HB2	39:j:41:ASN:HD21	1.59	0.65
44:p:343:TYR:CD2	44:p:344:ASN:OD1	2.49	0.65
6:C:157:HIS:NE2	6:C:179:ARG:CB	2.60	0.64
23:T:47:PRO:HB3	23:T:53:TRP:CD2	2.31	0.64
15:L:87:ARG:HG2	15:L:104:HIS:CE1	2.32	0.64
28:Y:5:ILE:HD11	28:Y:32:ARG:HD3	1.79	0.64
45:q:510:THR:HG23	45:q:514:LYS:HD2	1.78	0.64
36:g:138:VAL:O	36:g:138:VAL:HG12	1.97	0.64
3:A:81:TYR:CD2	3:A:167:LYS:CG	2.64	0.64
26:W:76:SER:CB	26:W:77:PRO:HD3	2.28	0.64
35:f:98:VAL:CG1	35:f:100:LEU:HD22	2.18	0.64
36:g:174:PHE:CD2	36:g:188:LEU:HD11	2.33	0.64
3:A:31:VAL:HG23	3:A:149:LEU:O	1.97	0.64
12:I:41:LYS:HG3	12:I:60:ILE:HD12	1.77	0.64
14:K:54:PHE:HD2	14:K:72:GLY:CA	2.07	0.64
35:f:99:LYS:HD2	35:f:99:LYS:N	2.11	0.64
35:f:119:LYS:HE2	35:f:120:GLU:OE2	1.96	0.64
39:j:93:GLU:O	39:j:97:LYS:HD3	1.98	0.64
2:2:477:A:H4'	13:J:127:VAL:HG21	1.79	0.64
2:2:512:U:H1'	13:J:131:GLN:HG3	1.79	0.64
2:2:1391:C:H5''	36:g:292:GLN:CD	2.23	0.64
2:2:750:U:H2'	2:2:751:G:H8	1.63	0.64
2:2:1290:G:H2'	2:2:1291:G:C8	2.32	0.64
3:A:197:ILE:HD13	3:A:202:TYR:OH	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:R:103:ASP:OD1	21:R:104:THR:HG23	1.98	0.64
38:i:45:GLY:O	38:i:60:HIS:HA	1.98	0.64
11:H:162:ILE:CG2	11:H:166:LEU:HD21	2.25	0.64
22:S:54:LEU:HD11	23:T:48:GLN:O	1.98	0.64
30:a:10:ARG:CA	30:a:34:LYS:HE2	2.28	0.64
39:j:20:VAL:HA	39:j:39:TYR:HE1	1.59	0.64
40:k:132:LEU:O	40:k:136:ILE:O	2.15	0.64
44:p:343:TYR:CE2	44:p:344:ASN:OD1	2.50	0.64
12:I:41:LYS:HA	12:I:59:ARG:C	2.15	0.64
44:p:363:LYS:O	44:p:364:ASN:HB3	1.98	0.64
11:H:89:HIS:ND1	11:H:165:LYS:HG2	2.12	0.64
39:j:121:ILE:HD13	39:j:121:ILE:H	1.63	0.64
48:l:101:7NO:O	40:k:381:PHE:HE1	1.80	0.63
36:g:268:LYS:HG2	36:g:280:GLU:HG2	1.80	0.63
23:T:47:PRO:CB	23:T:53:TRP:NE1	2.60	0.63
36:g:43:LEU:HD21	36:g:72:VAL:HG21	1.78	0.63
36:g:179:MET:CG	36:g:205:TYR:CD1	2.80	0.63
40:k:127:ARG:CD	40:k:133:GLU:HA	2.29	0.63
6:C:157:HIS:H	6:C:157:HIS:HD1	1.44	0.63
25:V:11:LEU:CD1	25:V:11:LEU:O	2.47	0.63
44:p:79:ILE:HD13	44:p:79:ILE:H	1.63	0.63
2:2:1726:U:H2'	2:2:1727:C:C6	2.34	0.63
26:W:31:SER:H	26:W:34:ILE:HD12	1.63	0.63
40:k:495:ILE:HG22	40:k:496:ASN:N	2.14	0.63
10:G:31:ARG:O	10:G:32:ILE:HB	1.99	0.63
10:G:32:ILE:HA	10:G:52:ILE:CG2	2.28	0.63
10:G:121:ILE:O	10:G:124:ILE:HG22	1.99	0.63
34:e:10:ARG:NH1	34:e:13:LYS:CG	2.45	0.63
39:j:20:VAL:HG12	39:j:39:TYR:CD1	2.33	0.63
8:E:238:LEU:HD12	8:E:242:LYS:NZ	2.14	0.63
36:g:179:MET:HB3	36:g:205:TYR:CE1	2.34	0.63
20:Q:99:GLU:HB3	36:g:58:PRO:HB2	1.79	0.63
11:H:98:ILE:CD1	11:H:121:VAL:HG11	2.27	0.63
23:T:34:VAL:HG13	23:T:54:PHE:CE2	2.32	0.63
29:Z:57:TYR:HE2	29:Z:59:TYR:CB	2.05	0.63
2:2:1191:C:H3'	2:2:1192:A:H5''	1.80	0.63
20:Q:109:PHE:HD1	20:Q:116:LEU:HD13	1.63	0.63
27:X:56:LYS:NZ	27:X:96:VAL:O	2.28	0.63
2:2:1536:U:H2'	2:2:1537:G:H3'	1.80	0.62
9:F:121:GLU:O	9:F:125:VAL:HG23	1.99	0.62
11:H:97:ARG:HG3	11:H:99:LEU:HG	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:I:41:LYS:HB2	12:I:60:ILE:HA	1.79	0.62
23:T:35:ASP:N	23:T:54:PHE:CE2	2.67	0.62
35:f:107:LYS:NZ	35:f:116:LYS:CA	2.61	0.62
14:K:87:PHE:HD2	14:K:91:TYR:CD1	2.17	0.62
36:g:62:TYR:OH	36:g:95:LEU:HA	1.98	0.62
42:m:34:ASN:HB2	42:m:37:LYS:HG3	1.80	0.62
43:o:702:UNK:O	43:o:703:UNK:C	2.47	0.62
14:K:54:PHE:CD2	14:K:72:GLY:CA	2.78	0.62
19:P:79:HIS:HA	19:P:97:TYR:HB3	1.81	0.62
25:V:12:TYR:HD1	25:V:13:VAL:N	1.98	0.62
27:X:34:LEU:O	27:X:39:LYS:CE	2.42	0.62
35:f:119:LYS:CD	35:f:120:GLU:H	2.07	0.62
36:g:288:TYR:HA	36:g:292:GLN:HE21	1.64	0.62
3:A:168:HIS:CG	3:A:203:PHE:CE2	2.88	0.62
8:E:21:ASP:OD1	8:E:25:GLY:N	2.32	0.62
8:E:65:LEU:HD23	8:E:77:ARG:O	1.99	0.62
12:I:36:THR:OG1	12:I:96:LEU:HB3	1.99	0.62
29:Z:52:LYS:O	29:Z:55:PRO:HD2	1.98	0.62
3:A:168:HIS:CG	3:A:203:PHE:HE2	2.18	0.62
42:m:74:MET:O	42:m:75:GLY:O	2.17	0.62
30:a:10:ARG:CA	30:a:34:LYS:CE	2.73	0.62
48:l:101:7NO:O	40:k:381:PHE:CE1	2.53	0.62
6:C:234:LEU:O	6:C:236:GLU:N	2.25	0.62
21:R:29:GLN:CB	36:g:86:TRP:CZ3	2.74	0.62
30:a:37:LYS:HD2	30:a:70:LYS:HE2	1.82	0.62
44:p:700:ARG:HA	44:p:711:LYS:CB	2.30	0.62
2:2:590:A:H2'	2:2:591:G:C8	2.34	0.62
3:A:92:HIS:HE1	3:A:202:TYR:OH	1.75	0.62
5:B:20:VAL:HB	5:B:23:PRO:HG3	1.82	0.62
22:S:12:GLN:OE1	22:S:12:GLN:N	2.33	0.62
33:d:34:TYR:CB	33:d:36:LEU:HD12	2.25	0.62
11:H:154:LEU:CD1	11:H:162:ILE:HG21	2.30	0.62
30:a:36:ILE:CD1	30:a:78:ALA:HB3	2.28	0.62
44:p:421:GLU:HG2	44:p:423:PRO:HD2	1.81	0.62
6:C:43:VAL:HG11	6:C:70:GLU:HB2	1.81	0.61
39:j:59:ILE:O	39:j:59:ILE:HD13	1.99	0.61
39:j:225:ALA:HB3	39:j:226:PRO:CD	2.26	0.61
2:2:453:U:H5'	8:E:62:LYS:HE2	1.81	0.61
7:D:16:VAL:CG2	33:d:22:ARG:NH1	2.46	0.61
14:K:87:PHE:CD2	14:K:91:TYR:CD1	2.88	0.61
18:O:61:MET:HG3	18:O:104:ALA:HB2	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:168:HIS:CA	3:A:203:PHE:HE2	2.10	0.61
13:J:39:LYS:HA	13:J:42:ILE:HD12	1.83	0.61
36:g:172:ILE:HG22	36:g:174:PHE:CE2	2.35	0.61
6:C:62:PHE:CD1	25:V:26:ALA:HB1	2.36	0.61
29:Z:57:TYR:CE2	29:Z:59:TYR:CB	2.81	0.61
2:2:311:A:H4'	2:2:312:U:H5'	1.82	0.61
3:A:197:ILE:CD1	3:A:202:TYR:OH	2.49	0.61
41:l:230:ILE:HA	41:l:234:VAL:HB	1.83	0.61
13:J:163:PRO:HG3	13:J:170:GLY:HA3	1.83	0.61
2:2:1712:A:H2'	2:2:1713:G:C8	2.35	0.61
8:E:11:ARG:HH12	8:E:20:LEU:HD22	1.66	0.61
30:a:22:ARG:HD2	30:a:28:ARG:O	2.00	0.61
2:2:485:G:H1	2:2:500:U:H3	1.48	0.61
20:Q:12:LYS:H	20:Q:83:GLN:HE21	1.47	0.61
22:S:12:GLN:H	22:S:59:GLY:C	2.09	0.61
3:A:26:ALA:HB1	3:A:149:LEU:HD22	1.82	0.61
25:V:11:LEU:HD12	25:V:11:LEU:O	2.00	0.61
39:j:74:LEU:HD22	39:j:89:ARG:NH1	2.15	0.61
44:p:360:ASP:HB2	44:p:364:ASN:O	2.00	0.61
9:F:45:PHE:O	9:F:71:TYR:O	2.19	0.61
20:Q:113:ASP:CA	20:Q:116:LEU:HD12	2.30	0.60
36:g:43:LEU:HB2	36:g:62:TYR:HB2	1.82	0.60
2:2:520:A:N3	28:Y:34:ASN:ND2	2.48	0.60
2:2:885:U:H2'	2:2:886:A:C8	2.37	0.60
16:M:28:SER:CB	16:M:34:LEU:HD11	2.31	0.60
28:Y:8:ARG:NH1	28:Y:28:LEU:HD11	2.17	0.60
29:Z:57:TYR:CD2	29:Z:59:TYR:N	2.69	0.60
28:Y:5:ILE:HD11	28:Y:32:ARG:HH11	1.63	0.60
30:a:36:ILE:O	30:a:73:TYR:HB2	2.01	0.60
6:C:147:GLY:CA	6:C:156:PRO:HB2	2.31	0.60
13:J:113:VAL:HG21	13:J:129:ILE:HD11	1.83	0.60
39:j:40:ASP:OD2	39:j:42:ILE:CG1	2.49	0.60
44:p:79:ILE:HD13	44:p:79:ILE:N	2.16	0.60
2:2:12:U:H1'	2:2:1298:G:H21	1.66	0.60
11:H:141:ARG:HG3	11:H:149:ILE:HB	1.84	0.60
36:g:5:ASN:OD1	36:g:325:ALA:HB3	2.02	0.60
38:i:56:LYS:C	38:i:56:LYS:HD3	2.25	0.60
38:i:58:MET:HB3	38:i:87:ASP:O	2.01	0.60
39:j:48:LEU:HD22	39:j:56:ILE:CD1	2.30	0.60
11:H:8:ILE:O	11:H:42:GLN:HA	2.02	0.60
11:H:162:ILE:HG22	11:H:166:LEU:CD2	2.28	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:k:127:ARG:NH1	40:k:136:ILE:H	2.00	0.60
41:l:135:LEU:HD23	41:l:135:LEU:C	2.27	0.60
6:C:43:VAL:HG13	6:C:44:THR:N	2.13	0.60
26:W:77:PRO:CB	27:X:9:LEU:HD23	2.32	0.60
30:a:28:ARG:HD2	30:a:74:CYS:SG	2.41	0.60
32:c:33:LEU:H	32:c:33:LEU:CD2	2.14	0.60
40:k:127:ARG:C	40:k:133:GLU:CG	2.75	0.60
44:p:700:ARG:CA	44:p:711:LYS:CB	2.80	0.60
26:W:3:ARG:CZ	26:W:28:ARG:NH2	2.64	0.60
33:d:21:CYS:CB	33:d:30:LEU:CD1	2.77	0.60
40:k:430:ILE:HD11	40:k:485:LEU:HB2	1.84	0.60
22:S:11:PHE:CA	22:S:59:GLY:C	2.74	0.59
32:c:33:LEU:HD23	32:c:33:LEU:N	2.17	0.59
36:g:154:LYS:CE	36:g:207:ASN:O	2.49	0.59
39:j:119:PHE:HB3	39:j:121:ILE:CD1	2.18	0.59
40:k:216:LEU:HD13	40:k:236:ILE:HD11	1.84	0.59
10:G:149:LYS:HG2	10:G:150:GLU:N	2.17	0.59
14:K:64:TYR:O	14:K:66:TYR:CE2	2.54	0.59
20:Q:33:GLY:O	20:Q:34:SER:OG	2.19	0.59
36:g:226:GLN:HB3	36:g:240:ASN:ND2	2.02	0.59
2:2:1043:U:H5	2:2:1074:C:H42	1.49	0.59
6:C:234:LEU:HD11	25:V:13:VAL:HG13	1.83	0.59
28:Y:35:VAL:CG2	28:Y:40:LEU:HD11	2.33	0.59
32:c:11:LYS:HB2	32:c:33:LEU:HB3	1.84	0.59
7:D:69:LEU:HA	7:D:72:LEU:HD12	1.83	0.59
20:Q:137:ARG:HB2	20:Q:137:ARG:NH1	2.17	0.59
24:U:107:THR:C	24:U:108:ILE:HD12	2.27	0.59
40:k:323:VAL:O	40:k:334:LYS:CG	2.45	0.59
2:2:69:G:H1	2:2:82:U:H3	1.50	0.59
38:i:55:ASN:OD1	38:i:57:ARG:CD	2.48	0.59
27:X:62:LYS:HD3	27:X:118:PRO:HG3	1.84	0.59
36:g:231:ASN:CG	36:g:234:HIS:CD2	2.76	0.59
1:1:48:5MC:H2'	1:1:59:A:H1'	1.83	0.59
2:2:309:C:O3'	27:X:24:TRP:HZ2	1.84	0.59
2:2:1711:G:H2'	2:2:1711:G:N3	2.18	0.59
11:H:46:ILE:HG13	11:H:60:VAL:HA	1.84	0.59
21:R:77:GLU:OE1	21:R:77:GLU:N	2.36	0.59
27:X:62:LYS:O	27:X:65:ASN:HB2	2.03	0.59
35:f:103:LEU:HD22	35:f:106:TYR:HE2	1.66	0.59
10:G:68:LEU:HG	10:G:101:ILE:HD11	1.84	0.59
24:U:22:ILE:HD13	24:U:100:VAL:CG1	2.08	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:59:TYR:CE1	30:a:62:TYR:HD1	2.21	0.59
36:g:154:LYS:CD	36:g:208:VAL:CG2	2.79	0.59
40:k:127:ARG:HD2	40:k:133:GLU:HA	1.85	0.59
44:p:390:LEU:CD2	44:p:477:ASP:O	2.50	0.59
21:R:27:ASP:OD2	36:g:20:TRP:CZ3	2.56	0.58
27:X:48:HIS:HB3	27:X:103:LEU:HD21	1.85	0.58
36:g:285:PHE:CE1	36:g:318:ARG:CZ	2.77	0.58
2:2:923:A:H2	2:2:987:A:H1'	1.67	0.58
16:M:28:SER:HB3	16:M:34:LEU:CD1	2.33	0.58
45:q:782:ASP:CG	45:q:783:GLU:H	2.11	0.58
2:2:31:C:H42	2:2:594:G:H1	1.51	0.58
2:2:1283:C:H4'	2:2:1285:U:H1'	1.85	0.58
6:C:86:MET:HB3	6:C:106:VAL:HG12	1.85	0.58
9:F:50:PHE:CE2	9:F:69:PRO:HA	2.38	0.58
27:X:40:SER:O	27:X:41:SER:OG	2.17	0.58
28:Y:28:LEU:HD12	28:Y:28:LEU:N	2.19	0.58
2:2:1312:A:H62	21:R:4:VAL:HB	1.69	0.58
9:F:153:GLY:HA3	9:F:158:ARG:HH11	1.67	0.58
19:P:63:ALA:HB1	19:P:74:ALA:H	1.68	0.58
2:2:1086:A:H2'	2:2:1087:A:H8	1.68	0.58
39:j:57:ARG:H	39:j:57:ARG:CD	2.09	0.58
2:2:1099:G:HO2'	26:W:76:SER:H	1.48	0.58
21:R:23:LYS:HG2	36:g:205:TYR:CE2	2.39	0.58
39:j:57:ARG:H	39:j:57:ARG:HH11	1.51	0.58
44:p:314:ILE:CD1	44:p:323:MET:CB	2.78	0.58
5:B:27:LYS:HB3	5:B:47:LEU:HD11	1.85	0.58
5:B:210:VAL:O	5:B:211:HIS:CG	2.56	0.58
14:K:54:PHE:HE2	14:K:75:TYR:CD1	2.20	0.58
20:Q:13:LYS:HG2	20:Q:79:TYR:CB	2.31	0.58
39:j:74:LEU:CD1	39:j:89:ARG:CZ	2.82	0.58
39:j:37:LEU:HB2	39:j:38:GLU:OE2	2.04	0.58
42:m:22:THR:C	42:m:24:ASN:N	2.62	0.58
7:D:76:ARG:CZ	14:K:22:VAL:HB	2.33	0.58
36:g:179:MET:HB3	36:g:205:TYR:CD1	2.39	0.58
2:2:385:G:H2'	2:2:386:A:C8	2.38	0.57
2:2:1251:C:H41	35:f:98:VAL:HB	1.68	0.57
8:E:191:ARG:HH22	8:E:216:ASN:HB3	1.69	0.57
10:G:123:GLY:O	10:G:127:ASP:N	2.36	0.57
15:L:129:ARG:HG2	15:L:130:PRO:HD2	1.86	0.57
21:R:110:VAL:O	21:R:114:GLY:CA	2.52	0.57
36:g:50:GLU:HG2	36:g:55:PHE:CE2	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:p:509:VAL:HG13	44:p:510:ALA:N	2.12	0.57
10:G:142:ARG:HE	10:G:149:LYS:HA	1.69	0.57
14:K:50:THR:O	14:K:53:GLY:HA2	2.04	0.57
32:c:13:ILE:HG23	32:c:14:LYS:HD3	1.83	0.57
35:f:107:LYS:HZ1	35:f:116:LYS:CA	2.17	0.57
2:2:980:U:H3	2:2:1019:A:H61	1.52	0.57
16:M:52:LEU:HD13	16:M:53:ALA:N	2.20	0.57
21:R:110:VAL:O	21:R:114:GLY:HA3	2.05	0.57
35:f:101:ALA:O	35:f:102:VAL:HG22	2.05	0.57
36:g:192:SER:O	36:g:194:ARG:HG3	2.04	0.57
38:i:60:HIS:HB2	38:i:88:GLN:OE1	2.02	0.57
1:1:13:C:H42	1:1:22:G:H1	1.52	0.57
12:I:152:LYS:C	12:I:153:ILE:HG13	2.29	0.57
18:O:92:LYS:O	18:O:93:THR:OG1	2.11	0.57
35:f:102:VAL:O	35:f:103:LEU:HD23	2.05	0.57
36:g:6:ILE:HG21	36:g:322:VAL:CG1	2.35	0.57
36:g:43:LEU:HD23	36:g:72:VAL:HG21	1.87	0.57
44:p:314:ILE:HD13	44:p:323:MET:CB	2.33	0.57
8:E:11:ARG:HG3	8:E:27:TYR:C	2.30	0.57
8:E:21:ASP:CG	8:E:24:SER:HB2	2.29	0.57
8:E:65:LEU:CD2	8:E:77:ARG:O	2.53	0.57
16:M:59:VAL:CG2	16:M:62:GLU:HA	2.34	0.57
22:S:13:HIS:C	22:S:14:ILE:HD12	2.29	0.57
40:k:127:ARG:HB3	40:k:133:GLU:CA	2.35	0.57
2:2:894:G:H1	2:2:916:U:H3	1.51	0.57
2:2:1377:C:H5''	2:2:1378:U:H5	1.69	0.57
21:R:23:LYS:CD	21:R:34:LEU:HD21	2.21	0.57
28:Y:31:ASN:ND2	28:Y:32:ARG:N	2.53	0.57
20:Q:35:PRO:HD2	20:Q:38:LEU:HB2	1.87	0.57
8:E:77:ARG:HG3	8:E:77:ARG:NH1	2.16	0.57
23:T:35:ASP:H	23:T:54:PHE:HZ	1.52	0.57
36:g:154:LYS:CE	36:g:208:VAL:CB	2.74	0.57
21:R:102:VAL:HG13	21:R:119:LEU:CD2	2.30	0.56
36:g:209:VAL:CG2	36:g:220:SER:HB3	2.30	0.56
43:o:298:LEU:HD21	43:o:352:TYR:HA	1.87	0.56
2:2:182:U:H3	2:2:201:A:H61	1.52	0.56
5:B:210:VAL:CG1	5:B:211:HIS:N	2.67	0.56
7:D:170:THR:HG23	7:D:187:LYS:HE2	1.88	0.56
21:R:77:GLU:O	21:R:81:LYS:NZ	2.34	0.56
36:g:154:LYS:CD	36:g:208:VAL:CB	2.83	0.56
40:k:277:GLY:O	40:k:278:ALA:CB	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:602:U:H2'	2:2:603:A:C8	2.40	0.56
7:D:124:ARG:HA	7:D:127:MET:HE3	1.87	0.56
8:E:179:LYS:HG3	8:E:231:PRO:HD3	1.87	0.56
8:E:238:LEU:HB2	8:E:242:LYS:HD2	1.86	0.56
16:M:37:GLY:H	16:M:110:SER:HB2	1.71	0.56
22:S:29:VAL:HG22	22:S:44:ASN:HA	1.87	0.56
22:S:101:LEU:O	22:S:105:LEU:HD23	2.04	0.56
29:Z:88:ILE:N	29:Z:88:ILE:HD12	2.20	0.56
30:a:23:CYS:HB3	30:a:27:SER:O	2.06	0.56
36:g:6:ILE:HG23	36:g:322:VAL:HG13	1.76	0.56
40:k:289:TYR:O	40:k:291:ILE:N	2.38	0.56
2:2:1198:G:H2'	2:2:1198:G:N3	2.20	0.56
7:D:74:GLU:HA	7:D:79:TYR:HB2	1.87	0.56
12:I:153:ILE:HG22	12:I:153:ILE:O	2.05	0.56
26:W:30:SER:CB	26:W:61:ILE:CG1	2.81	0.56
40:k:127:ARG:HB3	40:k:133:GLU:N	2.21	0.56
40:k:287:LEU:HD21	41:l:261:SER:O	2.06	0.56
22:S:13:HIS:O	22:S:24:GLY:N	2.38	0.56
42:m:67:ASN:HB2	42:m:79:GLN:HB3	1.88	0.56
10:G:14:LYS:HZ2	10:G:122:GLU:HB2	1.69	0.56
35:f:139:CYS:HB3	35:f:143:HIS:HA	1.87	0.56
2:2:1720:A:O2'	10:G:67:VAL:HA	2.06	0.56
11:H:26:ASP:O	11:H:29:ASN:ND2	2.38	0.56
11:H:97:ARG:C	11:H:97:ARG:HE	2.13	0.56
22:S:8:GLN:HA	22:S:57:ARG:NH1	2.21	0.56
22:S:12:GLN:O	22:S:59:GLY:HA3	2.06	0.56
9:F:82:LYS:HB3	9:F:85:ARG:HB2	1.86	0.56
21:R:104:THR:O	21:R:107:ALA:N	2.37	0.56
40:k:239:MET:O	40:k:240:LYS:HB2	2.04	0.56
44:p:228:ARG:N	44:p:231:TRP:CZ2	2.72	0.56
3:A:64:ILE:HG12	3:A:120:LEU:HD11	1.87	0.56
36:g:209:VAL:HG22	36:g:220:SER:HB2	1.84	0.56
39:j:73:VAL:HG13	39:j:84:ASP:O	2.06	0.56
40:k:124:GLN:HG2	40:k:126:VAL:H	1.71	0.56
44:p:79:ILE:HG12	44:p:129:VAL:O	2.06	0.56
2:2:1443:G:N1	35:f:90:LYS:O	2.39	0.55
2:2:1752:A:H4'	27:X:62:LYS:HG2	1.87	0.55
3:A:67:ILE:HD13	3:A:120:LEU:HD23	1.88	0.55
14:K:21:LEU:CD2	14:K:35:ILE:HD11	2.36	0.55
36:g:107:HIS:CA	36:g:133:ARG:NH2	2.68	0.55
36:g:157:VAL:HA	36:g:174:PHE:CD1	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:g:174:PHE:CD2	36:g:188:LEU:CG	2.89	0.55
45:q:106:GLU:O	45:q:110:LYS:N	2.25	0.55
22:S:28:VAL:O	22:S:29:VAL:HB	2.07	0.55
29:Z:39:ALA:O	29:Z:40:VAL:HG22	2.06	0.55
38:i:38:ILE:HD12	38:i:75:ASP:HB3	1.88	0.55
39:j:20:VAL:HG12	39:j:39:TYR:CG	2.41	0.55
39:j:74:LEU:HD22	39:j:89:ARG:HH12	1.70	0.55
43:o:707:UNK:O	43:o:711:UNK:N	2.39	0.55
14:K:54:PHE:HZ	14:K:75:TYR:CE1	2.24	0.55
36:g:126:ALA:CB	36:g:155:VAL:HG13	2.28	0.55
36:g:197:ALA:HB2	36:g:235:LYS:HE3	1.89	0.55
45:q:255:PHE:CD1	45:q:259:GLN:OE1	2.56	0.55
12:I:36:THR:OG1	12:I:96:LEU:CB	2.54	0.55
28:Y:5:ILE:HD11	28:Y:32:ARG:CD	2.36	0.55
30:a:57:SER:HB2	30:a:59:TYR:CE2	2.41	0.55
36:g:182:ILE:HG22	36:g:184:ARG:HG3	1.88	0.55
37:h:3:ALA:HA	37:h:6:ARG:HD3	1.87	0.55
41:l:204:SER:HB3	41:l:212:VAL:HB	1.88	0.55
44:p:363:LYS:O	44:p:364:ASN:CB	2.55	0.55
3:A:102:PHE:O	3:A:103:THR:HB	2.07	0.55
10:G:183:ARG:HA	10:G:186:ARG:HD2	1.89	0.55
11:H:170:GLN:HA	11:H:181:ILE:HD12	1.88	0.55
36:g:154:LYS:HZ3	36:g:208:VAL:HG21	1.70	0.55
39:j:28:ALA:HB3	39:j:32:ALA:N	2.17	0.55
2:2:1670:G:H2'	2:2:1671:G:C8	2.42	0.55
23:T:35:ASP:N	23:T:54:PHE:HE2	2.03	0.55
40:k:127:ARG:HB3	40:k:133:GLU:HA	1.88	0.55
13:J:169:PRO:HB2	13:J:174:ARG:HG3	1.89	0.55
16:M:110:SER:O	16:M:111:VAL:C	2.50	0.55
39:j:28:ALA:HB3	39:j:31:GLY:CA	2.34	0.55
8:E:11:ARG:NE	8:E:25:GLY:C	2.56	0.55
44:p:79:ILE:CD1	44:p:129:VAL:O	2.54	0.55
11:H:62:VAL:HG12	11:H:64:VAL:H	1.72	0.55
16:M:28:SER:HB3	16:M:34:LEU:HD12	1.89	0.55
25:V:40:ASP:CB	25:V:44:ARG:O	2.53	0.55
35:f:100:LEU:HD22	35:f:100:LEU:H	1.72	0.55
3:A:79:ARG:HG2	3:A:81:TYR:H	1.70	0.55
2:2:2:A:H5'	6:C:184:VAL:HG11	1.89	0.54
2:2:1433:G:O6	14:K:64:TYR:OH	2.25	0.54
30:a:36:ILE:HD13	30:a:84:VAL:CG2	2.37	0.54
2:2:897:A:H62	2:2:913:G:H21	1.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:167:LYS:O	3:A:170:ILE:CD1	2.54	0.54
36:g:157:VAL:CG2	36:g:174:PHE:CD1	2.70	0.54
36:g:179:MET:CB	36:g:205:TYR:HD1	2.20	0.54
42:m:22:THR:O	42:m:23:SER:C	2.49	0.54
2:2:1333:U:H3	2:2:1415:A:H61	1.55	0.54
20:Q:94:GLN:HE22	36:g:63:LYS:CE	2.20	0.54
30:a:59:TYR:HE1	30:a:62:TYR:CD1	2.25	0.54
33:d:31:ILE:CG1	33:d:38:ILE:H	2.19	0.54
41:l:139:PHE:C	41:l:142:LEU:HD13	2.31	0.54
3:A:81:TYR:O	3:A:167:LYS:HG2	2.07	0.54
9:F:56:LYS:HB2	9:F:140:ILE:HD13	1.88	0.54
9:F:65:GLN:OE1	9:F:90:PRO:CB	2.56	0.54
36:g:209:VAL:CG2	36:g:220:SER:CB	2.77	0.54
38:i:48:GLU:HG2	38:i:56:LYS:CE	2.38	0.54
40:k:136:ILE:HD13	40:k:137:THR:O	2.07	0.54
2:2:1557:A:H5''	22:S:135:GLY:HA3	1.90	0.54
2:2:1774:A:H2'	2:2:1775:G:C8	2.42	0.54
6:C:234:LEU:HD11	25:V:13:VAL:CG1	2.37	0.54
2:2:995:U:H3	2:2:1007:G:H1	1.56	0.54
2:2:1174:U:H2'	2:2:1175:G:H8	1.72	0.54
20:Q:130:GLY:C	20:Q:138:PHE:CE2	2.86	0.54
22:S:132:ARG:HH11	22:S:136:GLN:HE22	1.56	0.54
36:g:78:GLY:O	36:g:95:LEU:HD13	2.03	0.54
40:k:127:ARG:C	40:k:133:GLU:HG2	2.32	0.54
40:k:167:ASP:O	40:k:295:ASN:HB3	2.08	0.54
2:2:485:G:H2'	2:2:486:G:C8	2.42	0.54
5:B:24:PHE:HE2	5:B:27:LYS:HZ1	1.47	0.54
5:B:142:PHE:HB2	5:B:208:GLN:HB3	1.88	0.54
8:E:11:ARG:HG3	8:E:27:TYR:O	2.07	0.54
8:E:105:VAL:CB	8:E:244:ILE:O	2.54	0.54
3:A:168:HIS:CA	3:A:203:PHE:CZ	2.85	0.54
6:C:175:ILE:HB	6:C:202:TYR:HB2	1.89	0.54
10:G:216:LEU:HA	10:G:219:ARG:HE	1.72	0.54
11:H:46:ILE:HG23	11:H:59:ALA:O	2.07	0.54
23:T:35:ASP:CG	23:T:54:PHE:CE2	2.85	0.54
26:W:104:LEU:HB2	26:W:125:ILE:HA	1.90	0.54
42:m:93:ILE:HA	42:m:98:LEU:HB3	1.90	0.54
2:2:984:G:H1	2:2:1015:C:H42	1.55	0.54
12:I:21:PHE:CE1	12:I:22:ARG:HB3	2.42	0.54
24:U:51:VAL:HB	24:U:94:GLU:O	2.08	0.54
27:X:12:ALA:HA	27:X:15:LEU:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:j:46:ILE:HG21	39:j:87:LYS:HB2	1.89	0.54
7:D:200:LYS:HE2	7:D:200:LYS:C	2.33	0.54
21:R:20:TYR:C	21:R:22:PRO:HD2	2.32	0.54
22:S:8:GLN:HA	22:S:11:PHE:HE2	1.64	0.54
36:g:258:TRP:CG	36:g:278:ILE:CD1	2.91	0.54
36:g:276:VAL:HG12	36:g:277:LEU:N	2.23	0.54
44:p:306:LYS:O	44:p:310:HIS:ND1	2.42	0.54
2:2:14:C:H42	2:2:1139:G:H1	1.55	0.53
2:2:1397:C:H4'	2:2:1398:A:H5''	1.89	0.53
11:H:9:LEU:HD13	11:H:12:ALA:HB2	1.89	0.53
11:H:73:VAL:HG13	11:H:74:GLN:N	2.23	0.53
12:I:35:ASN:HB2	12:I:95:THR:CG2	2.37	0.53
18:O:64:ALA:HB1	18:O:105:LEU:HG	1.90	0.53
21:R:76:GLU:HB3	21:R:77:GLU:OE1	2.08	0.53
22:S:120:ARG:HE	22:S:125:ILE:HD11	1.72	0.53
32:c:34:GLU:H	32:c:34:GLU:CD	2.08	0.53
35:f:119:LYS:HE2	35:f:120:GLU:CD	2.33	0.53
43:o:97:ILE:HG22	43:o:185:LYS:HD2	1.89	0.53
11:H:89:HIS:CE1	11:H:165:LYS:HG2	2.42	0.53
29:Z:86:GLU:HB3	29:Z:88:ILE:HD11	1.90	0.53
38:i:55:ASN:CG	38:i:57:ARG:HG3	2.33	0.53
2:2:693:U:H3'	2:2:694:U:H5''	1.89	0.53
2:2:1087:A:C5	2:2:1088:U:H1'	2.43	0.53
24:U:82:TYR:HB3	33:d:52:PHE:HB3	1.91	0.53
36:g:14:LEU:HB2	36:g:317:ILE:HB	1.91	0.53
44:p:360:ASP:CB	44:p:364:ASN:O	2.56	0.53
8:E:44:LEU:HD11	8:E:72:VAL:HG21	1.90	0.53
14:K:54:PHE:CE2	14:K:72:GLY:HA2	2.42	0.53
11:H:8:ILE:HD12	11:H:21:ALA:HB1	1.89	0.53
11:H:126:LEU:HA	11:H:129:LEU:HD12	1.91	0.53
26:W:3:ARG:NH1	26:W:28:ARG:HH22	2.06	0.53
27:X:92:CYS:SG	27:X:95:PHE:CE1	3.02	0.53
30:a:44:ILE:HG22	30:a:65:PRO:O	2.09	0.53
36:g:238:PHE:O	36:g:239:MET:HG3	2.08	0.53
45:q:371:SER:HA	45:q:374:GLU:HB2	1.91	0.53
13:J:143:ILE:HG22	13:J:145:SER:H	1.73	0.53
22:S:28:VAL:HG21	22:S:54:LEU:HA	1.90	0.53
44:p:421:GLU:HG2	44:p:423:PRO:CD	2.39	0.53
45:q:510:THR:HG23	45:q:514:LYS:CD	2.39	0.53
2:2:111:U:H2'	2:2:112:A:C8	2.44	0.53
2:2:1657:A:H61	2:2:1740:U:H3	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:246:LEU:HD22	8:E:250:GLU:HG3	1.91	0.53
30:a:36:ILE:HD13	30:a:84:VAL:HG23	1.90	0.53
35:f:103:LEU:HD22	35:f:106:TYR:CE2	2.44	0.53
40:k:234:ALA:O	40:k:238:ILE:HG13	2.09	0.53
43:o:330:LEU:HD13	43:o:384:LEU:HD11	1.90	0.53
45:q:263:ASP:HB2	45:q:357:GLU:OE1	2.08	0.53
2:2:1634:C:H42	2:2:1765:G:H1	1.56	0.53
3:A:164:ASN:HB2	3:A:165:ARG:HH21	1.74	0.53
36:g:179:MET:CB	36:g:205:TYR:CD1	2.91	0.53
39:j:120:GLN:O	39:j:120:GLN:HG2	2.08	0.53
39:j:197:GLY:O	39:j:198:ILE:HG13	2.09	0.53
41:l:243:ASN:HB3	41:l:260:LYS:HB2	1.91	0.53
2:2:1443:G:N2	35:f:90:LYS:O	2.41	0.53
2:2:1685:U:H3	2:2:1712:A:H2	1.56	0.53
13:J:141:VAL:HG12	13:J:143:ILE:H	1.74	0.53
39:j:225:ALA:CB	39:j:226:PRO:CD	2.87	0.53
40:k:125:THR:CG2	40:k:137:THR:HG22	2.32	0.53
8:E:242:LYS:HG3	8:E:242:LYS:O	2.09	0.52
21:R:24:LEU:HD22	21:R:31:ASN:CG	2.34	0.52
22:S:119:ILE:C	22:S:119:ILE:HD12	2.34	0.52
25:V:11:LEU:CD1	25:V:11:LEU:C	2.82	0.52
28:Y:35:VAL:O	28:Y:36:SER:OG	2.27	0.52
29:Z:57:TYR:CD2	29:Z:59:TYR:C	2.87	0.52
30:a:36:ILE:CG1	30:a:75:ILE:HG22	2.39	0.52
3:A:41:ARG:HB3	3:A:43:ASP:OD1	2.10	0.52
7:D:137:VAL:HB	7:D:185:LYS:HB3	1.89	0.52
9:F:45:PHE:CE2	9:F:72:VAL:HA	2.44	0.52
12:I:38:ILE:N	12:I:38:ILE:HD12	2.24	0.52
25:V:12:TYR:CD1	25:V:12:TYR:C	2.87	0.52
42:m:92:MET:HE3	42:m:97:GLY:O	2.08	0.52
3:A:188:LEU:HD11	3:A:195:TRP:NE1	2.25	0.52
24:U:51:VAL:O	24:U:93:LEU:HD23	2.08	0.52
25:V:70:ASN:HB3	25:V:83:TRP:HB2	1.90	0.52
6:C:43:VAL:CG1	6:C:70:GLU:HB2	2.40	0.52
16:M:28:SER:HB2	16:M:34:LEU:HD11	1.89	0.52
18:O:87:GLY:HA3	18:O:120:PRO:HG2	1.91	0.52
22:S:123:ARG:HG3	22:S:133:VAL:HG11	1.92	0.52
31:b:2:VAL:HG23	31:b:3:LEU:N	2.16	0.52
33:d:19:ARG:CB	33:d:32:ARG:HH21	2.20	0.52
39:j:25:GLN:HE22	39:j:35:LYS:H	1.56	0.52
40:k:127:ARG:O	40:k:133:GLU:CD	2.53	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:p:214:TRP:HB2	44:p:223:SER:HA	1.92	0.52
2:2:107:C:H42	2:2:306:G:H1	1.56	0.52
23:T:46:PRO:O	23:T:47:PRO:C	2.50	0.52
29:Z:39:ALA:O	29:Z:40:VAL:HG23	2.08	0.52
29:Z:88:ILE:HD12	29:Z:88:ILE:H	1.75	0.52
36:g:151:TRP:CE3	36:g:179:MET:SD	3.03	0.52
43:o:261:GLU:HB3	43:o:351:MET:HE1	1.92	0.52
44:p:403:LEU:N	44:p:420:ALA:O	2.43	0.52
2:2:750:U:H2'	2:2:751:G:C8	2.44	0.52
2:2:1168:G:H21	2:2:1574:A:H62	1.58	0.52
18:O:24:ASN:ND2	18:O:24:ASN:H	2.07	0.52
22:S:11:PHE:CA	22:S:59:GLY:O	2.44	0.52
22:S:26:ILE:HG22	22:S:30:TYR:CB	2.33	0.52
36:g:289:THR:H	36:g:292:GLN:NE2	2.07	0.52
38:i:55:ASN:OD1	38:i:57:ARG:CG	2.57	0.52
40:k:452:LYS:HB2	44:p:293:ILE:HG21	1.92	0.52
44:p:421:GLU:OE1	44:p:424:ARG:HD2	2.10	0.52
2:2:41:A:H3'	2:2:437:A:H62	1.74	0.52
8:E:11:ARG:HA	8:E:28:ALA:HB2	1.90	0.52
15:L:16:GLN:HB3	15:L:19:ILE:HD13	1.92	0.52
30:a:10:ARG:O	30:a:11:ASN:HB3	2.10	0.52
36:g:112:LEU:HD11	36:g:128:ARG:CG	2.40	0.52
36:g:260:THR:HG23	36:g:301:TRP:CZ2	2.39	0.52
44:p:475:GLU:HB3	44:p:479:PRO:HG3	1.91	0.52
2:2:143:G:H2'	2:2:144:A:O4'	2.10	0.52
2:2:485:G:H2'	2:2:486:G:H8	1.74	0.52
2:2:1201:A:H62	2:2:1454:C:H3'	1.75	0.52
2:2:1637:C:H2'	2:2:1638:C:O4'	2.10	0.52
5:B:22:ASP:N	5:B:23:PRO:HD3	2.25	0.52
6:C:148:TYR:CE2	6:C:156:PRO:HD3	2.44	0.52
30:a:29:SER:O	30:a:30:VAL:C	2.53	0.52
3:A:55:GLU:O	3:A:58:VAL:HG12	2.09	0.52
3:A:85:ALA:HA	3:A:202:TYR:HB3	1.91	0.52
5:B:194:ASN:OD1	5:B:210:VAL:HG12	2.10	0.52
10:G:150:GLU:HA	10:G:150:GLU:OE2	2.08	0.52
13:J:99:LEU:O	13:J:100:LYS:HB2	2.10	0.52
44:p:282:LYS:HD2	44:p:345:ASP:OD2	2.10	0.52
45:q:652:ILE:HD12	45:q:655:SER:OG	2.10	0.52
2:2:506:U:H5'	2:2:507:U:H5''	1.92	0.52
2:2:627:G:H5'	17:N:120:SER:HB2	1.92	0.52
8:E:214:LEU:O	8:E:215:GLU:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:238:LEU:HD12	8:E:242:LYS:HZ2	1.74	0.52
12:I:36:THR:OG1	12:I:96:LEU:CA	2.57	0.52
28:Y:29:HIS:N	28:Y:30:PRO:HD3	2.24	0.52
36:g:47:ARG:HG3	36:g:59:VAL:CG1	2.39	0.52
36:g:154:LYS:HD2	36:g:208:VAL:CB	2.40	0.52
2:2:648:U:H3	2:2:685:A:H61	1.58	0.51
3:A:81:TYR:CB	3:A:167:LYS:HG3	2.38	0.51
8:E:73:ASP:O	8:E:164:LEU:HD21	2.10	0.51
30:a:10:ARG:CG	30:a:34:LYS:HE2	2.41	0.51
2:2:1236:G:H1	2:2:1247:C:H42	1.58	0.51
5:B:98:THR:H	5:B:232:HIS:HE1	1.57	0.51
11:H:162:ILE:H	11:H:162:ILE:HD12	1.74	0.51
22:S:11:PHE:C	22:S:11:PHE:CD1	2.88	0.51
23:T:69:LYS:HG3	23:T:70:GLN:HG2	1.91	0.51
36:g:202:HIS:ND1	36:g:228:TYR:CD2	2.77	0.51
39:j:226:PRO:CB	40:k:405:THR:HG22	2.41	0.51
2:2:569:A:N6	27:X:69:ARG:HH12	2.08	0.51
2:2:1475:G:H5'	23:T:43:ASN:HD21	1.74	0.51
14:K:87:PHE:CA	14:K:91:TYR:CD1	2.94	0.51
26:W:77:PRO:HB2	27:X:9:LEU:HD23	1.92	0.51
33:d:23:ILE:HG23	33:d:24:SER:N	2.25	0.51
39:j:59:ILE:HG23	39:j:60:GLN:HG2	1.92	0.51
41:l:232:GLU:O	41:l:268:VAL:HG11	2.09	0.51
45:q:630:ILE:H	45:q:631:PRO:HD2	1.76	0.51
2:2:523:U:N3	2:2:526:A:OP2	2.41	0.51
2:2:645:U:H2'	2:2:646:G:C8	2.45	0.51
5:B:35:PRO:HA	5:B:232:HIS:HD2	1.75	0.51
26:W:77:PRO:HB3	27:X:9:LEU:HD23	1.92	0.51
27:X:63:GLN:HB3	27:X:64:PRO:CD	2.40	0.51
35:f:105:TYR:HE2	35:f:106:TYR:CZ	2.23	0.51
2:2:559:U:H2'	2:2:560:G:C8	2.46	0.51
9:F:156:ALA:HB3	9:F:158:ARG:NH1	2.25	0.51
15:L:87:ARG:CZ	15:L:104:HIS:CB	2.82	0.51
29:Z:68:ARG:HH12	29:Z:70:LYS:HE3	1.74	0.51
35:f:101:ALA:C	35:f:102:VAL:HG13	2.35	0.51
44:p:219:ASN:HD22	44:p:219:ASN:N	2.07	0.51
44:p:228:ARG:HB2	44:p:231:TRP:HE1	0.57	0.51
44:p:532:THR:HG22	44:p:533:ASP:N	2.25	0.51
14:K:86:ILE:HG22	14:K:87:PHE:N	2.26	0.51
24:U:106:ILE:HD12	24:U:107:THR:H	1.74	0.51
33:d:32:ARG:O	33:d:32:ARG:HG2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:g:72:VAL:HG13	36:g:82:VAL:O	2.11	0.51
36:g:211:PRO:HD2	36:g:211:PRO:O	2.11	0.51
45:q:306:ALA:HB1	45:q:310:LEU:HD13	1.92	0.51
45:q:510:THR:CA	45:q:514:LYS:HD2	2.41	0.51
3:A:27:LYS:HA	3:A:45:VAL:HG22	1.91	0.51
6:C:227:TYR:HH	25:V:11:LEU:HD11	1.74	0.51
8:E:238:LEU:HD12	8:E:242:LYS:CE	2.41	0.51
10:G:32:ILE:O	10:G:34:GLN:HG3	2.11	0.51
18:O:17:ALA:O	18:O:81:ILE:HA	2.10	0.51
19:P:126:VAL:O	19:P:127:ARG:NE	2.35	0.51
21:R:10:LYS:HE2	21:R:10:LYS:HA	1.93	0.51
22:S:29:VAL:HG13	22:S:43:ALA:CB	2.40	0.51
29:Z:39:ALA:C	29:Z:40:VAL:HG23	2.36	0.51
35:f:100:LEU:CD2	35:f:100:LEU:H	2.23	0.51
44:p:509:VAL:CG1	44:p:510:ALA:H	2.09	0.51
2:2:291:U:H2'	2:2:292:U:C6	2.46	0.51
2:2:702:G:H1	2:2:736:C:H42	1.58	0.51
2:2:1079:U:O4	2:2:1090:A:N1	2.44	0.51
8:E:106:LYS:HA	8:E:245:LYS:CE	2.40	0.51
9:F:123:ILE:HB	9:F:131:PRO:HB3	1.92	0.51
12:I:113:TYR:CE1	12:I:153:ILE:HD11	2.44	0.51
17:N:15:ALA:HB2	31:b:20:LYS:HD3	1.92	0.51
25:V:55:LEU:HB3	25:V:59:ILE:HD11	1.93	0.51
43:o:287:VAL:HG11	43:o:303:TRP:HD1	1.76	0.51
2:2:70:C:H2'	2:2:71:A:O4'	2.11	0.51
16:M:29:LEU:HD11	16:M:92:ALA:HA	1.93	0.51
18:O:81:ILE:HB	18:O:115:ILE:HG22	1.93	0.51
24:U:45:ALA:O	24:U:49:LYS:N	2.43	0.51
28:Y:15:ASN:HB3	28:Y:20:ARG:HG3	1.93	0.51
36:g:272:LEU:N	36:g:272:LEU:CD1	2.73	0.51
2:2:654:G:H2'	2:2:655:G:H8	1.75	0.51
2:2:1047:G:H1	2:2:1069:C:H42	1.58	0.51
16:M:28:SER:O	16:M:32:ASP:N	2.44	0.51
19:P:91:GLY:HA2	19:P:106:GLU:OE1	2.10	0.51
21:R:103:ASP:O	21:R:106:THR:HG22	2.11	0.51
28:Y:105:ARG:HH21	28:Y:109:LYS:HE3	1.75	0.51
45:q:613:ASN:HB3	45:q:616:LEU:HB2	1.93	0.51
12:I:153:ILE:HB	12:I:158:ASP:OD1	2.10	0.50
45:q:357:GLU:O	45:q:357:GLU:HG2	2.12	0.50
2:2:889:C:H42	2:2:921:G:H1	1.60	0.50
2:2:1392:G:OP2	36:g:292:GLN:NE2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:31:VAL:CG2	3:A:149:LEU:O	2.58	0.50
5:B:24:PHE:CD2	5:B:27:LYS:NZ	2.73	0.50
14:K:58:GLN:HB2	14:K:65:TYR:HB2	1.92	0.50
14:K:88:PRO:CD	14:K:91:TYR:CE1	2.94	0.50
30:a:63:ALA:O	30:a:64:LEU:HB3	2.12	0.50
40:k:127:ARG:CB	40:k:133:GLU:HG2	2.41	0.50
42:m:48:GLU:HB2	42:m:96:LEU:HG	1.93	0.50
2:2:1180:U:O2'	19:P:128:HIS:CE1	2.65	0.50
36:g:35:VAL:HG21	36:g:74:VAL:CG2	2.41	0.50
36:g:126:ALA:HB1	36:g:152:VAL:HG11	1.91	0.50
40:k:136:ILE:CB	51:k:602:GCP:H3B1	2.41	0.50
2:2:628:U:H2'	2:2:629:A:H8	1.75	0.50
25:V:8:LEU:HD21	25:V:10:GLU:HB3	1.93	0.50
27:X:14:LYS:O	27:X:17:VAL:HG12	2.11	0.50
36:g:151:TRP:CE3	36:g:179:MET:CE	2.94	0.50
45:q:510:THR:HG22	45:q:514:LYS:HD2	1.93	0.50
48:l:101:7NO:C8	40:k:323:VAL:HG23	2.42	0.50
2:2:891:A:H61	2:2:919:U:H3	1.58	0.50
2:2:965:A:H2'	2:2:966:A:C8	2.47	0.50
3:A:175:TYR:HD1	3:A:202:TYR:HE2	1.60	0.50
10:G:123:GLY:HA3	10:G:127:ASP:HB2	1.94	0.50
35:f:98:VAL:HG11	35:f:100:LEU:HD21	1.90	0.50
36:g:209:VAL:HG22	36:g:220:SER:CA	2.40	0.50
43:o:714:UNK:O	43:o:718:UNK:N	2.44	0.50
21:R:113:LEU:O	21:R:113:LEU:HD23	2.12	0.50
29:Z:80:LEU:HD23	29:Z:81:ARG:HG3	1.93	0.50
36:g:151:TRP:HE3	36:g:179:MET:CE	2.23	0.50
44:p:228:ARG:CB	44:p:231:TRP:NE1	2.33	0.50
2:2:328:G:H2'	2:2:329:G:C8	2.47	0.50
9:F:185:ALA:CB	9:F:192:ILE:HG12	2.42	0.50
14:K:87:PHE:HA	14:K:91:TYR:HE1	1.68	0.50
27:X:63:GLN:C	27:X:65:ASN:N	2.70	0.50
29:Z:57:TYR:HD2	29:Z:59:TYR:C	2.19	0.50
2:2:1108:G:H2'	2:2:1109:G:H8	1.77	0.50
2:2:1269:G:H1'	2:2:1445:C:H6	1.76	0.50
2:2:1499:C:H42	2:2:1504:G:H1	1.60	0.50
14:K:50:THR:O	14:K:53:GLY:N	2.45	0.50
21:R:25:THR:HG22	21:R:26:MET:HG2	1.94	0.50
24:U:71:PRO:HB3	33:d:41:GLN:HG3	1.92	0.50
35:f:119:LYS:HE3	35:f:120:GLU:OE1	2.12	0.50
40:k:148:TYR:H	40:k:168:LYS:HA	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:q:356:LYS:O	45:q:357:GLU:HB2	2.12	0.50
3:A:41:ARG:C	3:A:43:ASP:H	2.19	0.50
10:G:88:ARG:HB3	10:G:88:ARG:HH11	1.75	0.50
11:H:63:PRO:O	11:H:64:VAL:HB	2.12	0.50
14:K:53:GLY:C	14:K:54:PHE:HD1	2.20	0.50
14:K:55:VAL:HG12	14:K:56:LYS:N	2.27	0.50
36:g:283:PRO:HB2	36:g:285:PHE:CE2	2.46	0.50
38:i:55:ASN:HD22	38:i:56:LYS:N	2.09	0.50
40:k:136:ILE:HB	51:k:602:GCP:H3B1	1.93	0.50
45:q:500:LYS:HB3	45:q:539:LEU:HD21	1.93	0.50
2:2:648:U:H3	2:2:685:A:N6	2.09	0.49
2:2:996:G:H1	2:2:1006:C:H42	1.60	0.49
9:F:50:PHE:HE2	9:F:69:PRO:HA	1.74	0.49
12:I:41:LYS:HB2	12:I:60:ILE:HD12	1.93	0.49
13:J:120:LYS:C	13:J:121:SER:HG	2.20	0.49
16:M:37:GLY:H	16:M:110:SER:CB	2.24	0.49
20:Q:69:VAL:HG21	20:Q:81:ILE:HG12	1.93	0.49
26:W:76:SER:HB3	26:W:77:PRO:CD	2.37	0.49
30:a:13:LYS:H	30:a:15:ARG:CZ	2.25	0.49
36:g:154:LYS:CD	36:g:208:VAL:CA	2.68	0.49
2:2:510:A:C8	13:J:172:VAL:HG11	2.47	0.49
5:B:24:PHE:HE2	5:B:27:LYS:NZ	2.07	0.49
5:B:191:GLU:HB2	5:B:194:ASN:HD22	1.76	0.49
8:E:128:LYS:HE2	8:E:130:GLN:HE21	1.77	0.49
10:G:32:ILE:HG22	10:G:33:GLY:N	2.26	0.49
30:a:12:LYS:CA	30:a:15:ARG:HH21	2.03	0.49
36:g:289:THR:OG1	36:g:292:GLN:CG	2.58	0.49
44:p:412:ASN:HD22	44:p:412:ASN:C	2.20	0.49
2:2:728:A:H2'	2:2:728:A:N3	2.27	0.49
2:2:1141:A:H2'	2:2:1142:A:C8	2.47	0.49
6:C:142:ILE:HG21	6:C:224:GLY:HA2	1.93	0.49
12:I:103:GLN:HB3	12:I:165:ARG:HD2	1.93	0.49
12:I:168:ALA:HB2	12:I:184:ILE:HD12	1.94	0.49
16:M:68:VAL:HG21	16:M:111:VAL:HG21	1.94	0.49
39:j:226:PRO:HB3	40:k:405:THR:HG22	1.95	0.49
40:k:355:ILE:HG22	40:k:357:PRO:HD2	1.94	0.49
44:p:79:ILE:CD1	44:p:130:GLU:HA	2.42	0.49
1:1:16:H2U:H52	39:j:103:GLN:HE21	1.78	0.49
2:2:127:G:H21	2:2:177:U:H3	1.59	0.49
7:D:194:ARG:O	7:D:196:THR:N	2.45	0.49
10:G:123:GLY:HA2	10:G:126:ASN:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:K:77:ARG:HH21	14:K:86:ILE:HD13	1.78	0.49
26:W:79:PHE:H	26:W:125:ILE:HG22	1.77	0.49
28:Y:29:HIS:HD2	28:Y:34:ASN:C	1.91	0.49
36:g:29:ALA:HB3	36:g:77:ASP:C	2.37	0.49
36:g:138:VAL:O	36:g:138:VAL:CG1	2.60	0.49
5:B:98:THR:H	5:B:232:HIS:CE1	2.30	0.49
9:F:66:ILE:H	9:F:91:ILE:HD11	1.77	0.49
22:S:7:GLU:O	22:S:8:GLN:HG3	2.12	0.49
22:S:91:ASP:OD2	22:S:93:ASN:HB2	2.11	0.49
30:a:13:LYS:H	30:a:15:ARG:NH2	2.11	0.49
39:j:188:VAL:HG22	39:j:264:ILE:HA	1.94	0.49
16:M:52:LEU:HD21	16:M:80:ILE:HD12	1.93	0.49
21:R:29:GLN:CB	36:g:86:TRP:HZ3	2.18	0.49
27:X:20:ARG:C	27:X:24:TRP:HD1	2.12	0.49
28:Y:18:LEU:HB2	28:Y:20:ARG:HG2	1.95	0.49
43:o:200:LYS:HG3	43:o:252:LEU:HD22	1.94	0.49
2:2:9:U:H2'	2:2:11:A:N7	2.28	0.49
12:I:29:LEU:HD22	12:I:29:LEU:C	2.37	0.49
14:K:88:PRO:CD	14:K:91:TYR:HE1	2.24	0.49
18:O:25:ASP:HA	18:O:54:GLU:HB3	1.95	0.49
23:T:70:GLN:HB3	23:T:121:GLY:HA3	1.94	0.49
24:U:27:THR:HG23	24:U:88:LYS:HG2	1.93	0.49
35:f:100:LEU:CD2	35:f:100:LEU:N	2.75	0.49
36:g:72:VAL:HG12	36:g:73:VAL:N	2.28	0.49
44:p:531:LYS:HG3	44:p:532:THR:H	1.78	0.49
2:2:1592:G:H5'	33:d:33:LYS:HD2	1.94	0.49
2:2:1650:C:H2'	2:2:1651:C:C6	2.48	0.49
6:C:235:TRP:CZ2	26:W:68:ARG:HB3	2.48	0.49
8:E:163:ASP:O	8:E:167:GLY:N	2.44	0.49
14:K:87:PHE:CE2	14:K:91:TYR:CD2	3.01	0.49
22:S:92:VAL:HG13	22:S:93:ASN:OD1	2.13	0.49
33:d:30:LEU:HD22	33:d:30:LEU:N	2.26	0.49
34:e:10:ARG:HH11	34:e:13:LYS:HG2	1.64	0.49
40:k:289:TYR:O	40:k:291:ILE:CG1	2.60	0.49
44:p:481:GLU:OE1	44:p:536:LYS:O	2.30	0.49
2:2:512:U:O2	2:2:512:U:O4'	2.31	0.49
2:2:965:A:H2'	2:2:966:A:H8	1.78	0.49
2:2:1752:A:H5'	27:X:62:LYS:HD2	1.94	0.49
7:D:195:ASN:O	7:D:196:THR:HB	2.13	0.49
11:H:154:LEU:HD13	11:H:162:ILE:HG21	1.95	0.49
2:2:674:A:H2'	2:2:674:A:N3	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1243:A:H2'	2:2:1243:A:N3	2.28	0.48
2:2:1588:G:H1	2:2:1604:C:H42	1.60	0.48
2:2:1715:G:H2'	2:2:1716:A:C8	2.48	0.48
12:I:22:ARG:HG2	12:I:22:ARG:HH11	1.77	0.48
21:R:23:LYS:HG2	36:g:205:TYR:CZ	2.47	0.48
23:T:102:ARG:HA	23:T:105:LEU:HD12	1.94	0.48
24:U:44:ASN:O	24:U:48:PHE:HD2	1.96	0.48
30:a:25:ASN:HD22	30:a:77:CYS:CB	2.26	0.48
36:g:104:PHE:CE2	36:g:139:GLY:HA2	2.48	0.48
45:q:642:VAL:HG12	45:q:763:LEU:HD12	1.94	0.48
2:2:1191:C:C3'	2:2:1192:A:H5''	2.43	0.48
10:G:68:LEU:O	10:G:101:ILE:CG1	2.59	0.48
13:J:56:ALA:HA	13:J:59:LEU:HD12	1.94	0.48
14:K:87:PHE:CB	14:K:91:TYR:CD1	2.96	0.48
19:P:71:GLU:O	19:P:72:LYS:HB3	2.13	0.48
22:S:29:VAL:O	22:S:33:THR:CG2	2.56	0.48
36:g:46:TRP:CZ3	36:g:58:PRO:HG3	2.47	0.48
44:p:461:GLY:O	44:p:462:LYS:HB3	2.13	0.48
1:1:64:RIA:N3	1:1:64:RIA:H2A	2.29	0.48
2:2:1477:A:H61	2:2:1526:U:H3	1.61	0.48
6:C:234:LEU:O	6:C:236:GLU:HG3	2.11	0.48
26:W:14:ILE:HD11	26:W:27:ILE:HD11	1.95	0.48
28:Y:21:LYS:HB2	28:Y:75:VAL:HB	1.95	0.48
29:Z:68:ARG:HH12	29:Z:70:LYS:HE2	1.77	0.48
36:g:154:LYS:NZ	36:g:248:PHE:O	2.46	0.48
36:g:258:TRP:CG	36:g:278:ILE:HD11	2.47	0.48
43:o:45:PRO:HG3	43:o:79:ILE:HG12	1.96	0.48
3:A:31:VAL:HG12	3:A:33:GLN:H	1.78	0.48
3:A:191:ARG:HD2	25:V:43:GLY:HA2	1.94	0.48
6:C:145:ARG:HH12	6:C:231:THR:HG21	1.79	0.48
24:U:95:ALA:HB1	24:U:99:ILE:HD11	1.95	0.48
26:W:75:ILE:HG21	26:W:125:ILE:HG23	1.96	0.48
28:Y:60:PHE:CD1	28:Y:71:GLY:HA3	2.47	0.48
30:a:51:ARG:HG3	30:a:55:GLU:OE2	2.13	0.48
40:k:210:VAL:HG22	40:k:341:SER:HB3	1.95	0.48
43:o:713:UNK:O	43:o:717:UNK:N	2.46	0.48
45:q:782:ASP:OD1	45:q:783:GLU:N	2.44	0.48
2:2:27:U:H2'	2:2:28:A:C8	2.49	0.48
2:2:1506:U:H2'	2:2:1507:C:C6	2.49	0.48
3:A:92:HIS:CE1	3:A:202:TYR:CZ	2.98	0.48
8:E:105:VAL:HB	8:E:244:ILE:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:14:LYS:HE3	10:G:122:GLU:HG2	1.96	0.48
12:I:78:ILE:HG23	12:I:102:VAL:HG21	1.95	0.48
31:b:59:CYS:SG	31:b:61:THR:HG23	2.54	0.48
32:c:32:PHE:HB3	32:c:34:GLU:OE1	2.13	0.48
2:2:569:A:H61	27:X:69:ARG:HH12	1.62	0.48
2:2:869:C:O2'	31:b:51:GLN:HB3	2.14	0.48
10:G:67:VAL:O	10:G:68:LEU:HB3	2.14	0.48
12:I:81:VAL:HG12	12:I:91:VAL:HG13	1.95	0.48
26:W:57:ARG:HG3	26:W:57:ARG:O	2.13	0.48
28:Y:15:ASN:HB2	28:Y:22:GLN:HE21	1.79	0.48
32:c:32:PHE:CD2	32:c:38:ARG:HB2	2.48	0.48
34:e:10:ARG:HE	34:e:13:LYS:HA	1.79	0.48
40:k:246:ILE:HD12	40:k:270:ILE:HG12	1.95	0.48
42:m:45:VAL:HB	42:m:76:GLU:HB3	1.96	0.48
43:o:40:ILE:HB	43:o:78:LEU:HD21	1.96	0.48
44:p:339:VAL:HG22	44:p:350:ARG:HG3	1.96	0.48
9:F:26:GLU:HG2	9:F:36:GLN:HE22	1.78	0.48
11:H:126:LEU:O	11:H:129:LEU:HB2	2.14	0.48
22:S:11:PHE:CB	22:S:59:GLY:C	2.85	0.48
27:X:50:LYS:HG3	27:X:103:LEU:HD23	1.96	0.48
27:X:51:GLY:HA2	27:X:77:ILE:HG13	1.95	0.48
27:X:63:GLN:HB3	27:X:64:PRO:HD2	1.95	0.48
30:a:44:ILE:CG2	30:a:65:PRO:O	2.62	0.48
36:g:252:PHE:HE1	36:g:272:LEU:HD21	1.77	0.48
43:o:283:TYR:HA	43:o:286:LEU:HD12	1.95	0.48
13:J:120:LYS:O	13:J:124:HIS:HB3	2.13	0.48
40:k:98:GLN:HG3	40:k:391:VAL:HB	1.93	0.48
40:k:127:ARG:C	40:k:133:GLU:HG3	2.39	0.48
2:2:1531:C:H4'	2:2:1537:G:C6	2.49	0.48
19:P:68:PRO:O	19:P:70:ASN:OD1	2.32	0.48
21:R:41:ILE:HD13	21:R:47:ARG:HG2	1.95	0.48
23:T:39:THR:HG21	23:T:54:PHE:CZ	2.48	0.48
30:a:36:ILE:HD11	30:a:75:ILE:HG22	1.96	0.48
36:g:289:THR:HG1	36:g:292:GLN:HG2	1.78	0.48
44:p:79:ILE:HD11	44:p:130:GLU:HA	1.95	0.48
44:p:112:MET:HB3	44:p:127:LEU:HD11	1.96	0.48
44:p:421:GLU:CG	44:p:423:PRO:HD2	2.44	0.48
2:2:558:C:H42	2:2:585:G:H1	1.59	0.48
2:2:1332:C:H42	2:2:1416:G:H1	1.62	0.48
2:2:1774:A:H2'	2:2:1775:G:H8	1.78	0.48
14:K:92:LEU:HD23	14:K:93:ALA:CA	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:62:TYR:OH	30:a:65:PRO:HD3	2.14	0.48
36:g:43:LEU:HD21	36:g:72:VAL:HG22	1.93	0.48
2:2:5:U:H2'	2:2:6:G:C8	2.48	0.47
2:2:327:A:H2'	2:2:328:G:C8	2.48	0.47
2:2:1139:G:H2'	2:2:1140:G:H8	1.77	0.47
5:B:134:VAL:HG12	5:B:218:LEU:HB2	1.96	0.47
12:I:21:PHE:O	12:I:22:ARG:CG	2.49	0.47
14:K:61:TRP:C	14:K:62:GLN:HG2	2.38	0.47
14:K:86:ILE:HD12	14:K:86:ILE:N	2.29	0.47
16:M:34:LEU:HD12	16:M:34:LEU:N	2.29	0.47
21:R:102:VAL:CG1	21:R:119:LEU:HD22	2.35	0.47
22:S:26:ILE:CG2	22:S:30:TYR:CB	2.91	0.47
28:Y:36:SER:OG	28:Y:39:GLU:HB2	2.14	0.47
33:d:36:LEU:HD22	33:d:38:ILE:HD11	1.95	0.47
35:f:105:TYR:CZ	35:f:106:TYR:CZ	3.00	0.47
36:g:272:LEU:CD1	36:g:272:LEU:H	2.27	0.47
39:j:209:GLU:HA	39:j:218:VAL:HA	1.96	0.47
45:q:335:THR:HG22	45:q:335:THR:O	2.13	0.47
2:2:142:G:H2'	2:2:143:G:C8	2.49	0.47
2:2:1191:C:H5''	2:2:1192:A:H5''	1.97	0.47
8:E:94:ALA:HB1	28:Y:16:PRO:HB2	1.95	0.47
9:F:45:PHE:CD2	9:F:71:TYR:O	2.67	0.47
14:K:61:TRP:O	14:K:63:TYR:CD2	2.67	0.47
25:V:12:TYR:CD1	25:V:13:VAL:N	2.80	0.47
28:Y:2:SER:N	28:Y:31:ASN:OD1	2.46	0.47
2:2:13:C:H4'	2:2:1297:U:H1'	1.97	0.47
2:2:935:G:H1	2:2:942:C:H42	1.61	0.47
2:2:939:A:H2'	2:2:940:A:H8	1.79	0.47
2:2:1346:U:H1'	2:2:1515:U:H1'	1.96	0.47
2:2:1458:A:N9	19:P:129:GLY:HA3	2.29	0.47
3:A:76:ILE:HD12	3:A:121:VAL:HG13	1.96	0.47
3:A:81:TYR:CD2	3:A:167:LYS:HD3	2.49	0.47
3:A:88:LYS:HD3	3:A:202:TYR:HE1	1.62	0.47
13:J:129:ILE:HG12	13:J:134:ILE:HD13	1.96	0.47
22:S:57:ARG:HB2	22:S:60:GLU:HB2	1.95	0.47
24:U:108:ILE:HD12	24:U:108:ILE:N	2.29	0.47
28:Y:8:ARG:NH2	28:Y:28:LEU:CD1	2.78	0.47
36:g:160:LYS:NZ	36:g:173:THR:OG1	2.36	0.47
39:j:28:ALA:HB3	39:j:31:GLY:O	2.12	0.47
41:l:173:ILE:HG12	41:l:212:VAL:HG22	1.95	0.47
44:p:314:ILE:HD12	44:p:323:MET:CB	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:560:G:H1	2:2:583:C:H42	1.61	0.47
2:2:941:G:H5'	2:2:976:A:H4'	1.97	0.47
2:2:1116:U:H2'	2:2:1117:G:O4'	2.14	0.47
2:2:1290:G:H2'	2:2:1291:G:H8	1.79	0.47
3:A:183:ARG:HD3	3:A:191:ARG:HG2	1.97	0.47
12:I:47:ARG:HG3	12:I:53:GLN:HE21	1.80	0.47
24:U:46:GLU:O	24:U:49:LYS:CE	2.62	0.47
39:j:119:PHE:O	39:j:120:GLN:HB3	2.15	0.47
44:p:540:LEU:HD21	44:p:543:GLU:HB2	1.96	0.47
2:2:50:C:H42	2:2:428:G:H1	1.62	0.47
2:2:111:U:H2'	2:2:112:A:H8	1.80	0.47
2:2:813:A:N3	2:2:813:A:H2'	2.30	0.47
3:A:73:VAL:HA	3:A:120:LEU:HB3	1.97	0.47
5:B:117:TRP:CE3	5:B:153:THR:HG21	2.37	0.47
8:E:105:VAL:O	8:E:245:LYS:HB2	2.15	0.47
10:G:68:LEU:C	10:G:101:ILE:HG13	2.39	0.47
23:T:10:PRO:HB2	23:T:13:ASP:HB3	1.97	0.47
27:X:102:VAL:HG23	27:X:127:VAL:HA	1.95	0.47
29:Z:57:TYR:CE2	29:Z:59:TYR:CA	2.98	0.47
30:a:78:ALA:HA	30:a:83:ILE:HD12	1.96	0.47
36:g:174:PHE:CE2	36:g:188:LEU:CG	2.94	0.47
40:k:233:LEU:HD11	40:k:273:THR:HG22	1.96	0.47
2:2:55:A:H3'	2:2:402:G:H1	1.79	0.47
20:Q:109:PHE:CD1	20:Q:116:LEU:HD13	2.48	0.47
26:W:75:ILE:HG21	26:W:125:ILE:CG2	2.45	0.47
30:a:36:ILE:CD1	30:a:75:ILE:HA	2.39	0.47
30:a:64:LEU:C	30:a:64:LEU:CD2	2.86	0.47
39:j:28:ALA:CA	39:j:31:GLY:O	2.62	0.47
2:2:125:U:H3	2:2:290:G:H22	1.61	0.47
2:2:327:A:H2'	2:2:328:G:H8	1.78	0.47
2:2:328:G:H2'	2:2:329:G:H8	1.78	0.47
2:2:1170:A:H2'	2:2:1171:G:C8	2.49	0.47
2:2:1261:U:H2'	2:2:1262:G:H8	1.80	0.47
5:B:71:ALA:HB2	5:B:80:SER:HA	1.96	0.47
5:B:117:TRP:HB3	5:B:153:THR:CG2	2.41	0.47
7:D:65:ARG:O	7:D:68:GLU:HG3	2.15	0.47
8:E:105:VAL:HG12	8:E:244:ILE:H	1.80	0.47
8:E:201:HIS:HB2	8:E:205:PHE:O	2.14	0.47
10:G:149:LYS:O	10:G:150:GLU:HB2	2.15	0.47
11:H:55:LYS:HE2	11:H:87:ASP:CG	2.39	0.47
11:H:129:LEU:HB3	11:H:169:PHE:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:I:41:LYS:HG3	12:I:60:ILE:CD1	2.43	0.47
16:M:52:LEU:CD1	16:M:54:VAL:HG23	2.45	0.47
16:M:120:ASP:OD2	16:M:124:ARG:CD	2.61	0.47
22:S:100:SER:HB2	22:S:105:LEU:HB3	1.97	0.47
30:a:62:TYR:CZ	30:a:65:PRO:HD3	2.49	0.47
30:a:64:LEU:HD23	30:a:64:LEU:O	2.13	0.47
44:p:226:GLU:O	44:p:231:TRP:HH2	1.97	0.47
9:F:133:GLN:O	9:F:136:VAL:HG12	2.15	0.47
11:H:9:LEU:HD23	11:H:43:PHE:HB2	1.97	0.47
22:S:11:PHE:CB	22:S:60:GLU:N	2.73	0.47
45:q:554:ALA:HB1	45:q:559:LEU:HB3	1.95	0.47
2:2:601:U:H2'	2:2:602:U:C6	2.49	0.47
2:2:765:G:C6	13:J:146:PHE:HZ	2.32	0.47
2:2:765:G:H1	13:J:149:ARG:HB2	1.80	0.47
7:D:7:LYS:HB3	24:U:27:THR:HG21	1.97	0.47
9:F:144:PRO:HG3	9:F:216:LYS:HE2	1.97	0.47
21:R:24:LEU:HD13	21:R:54:THR:HG21	1.96	0.47
26:W:11:LEU:HD12	26:W:74:VAL:HG23	1.96	0.47
39:j:74:LEU:O	39:j:75:ARG:HB2	2.15	0.47
5:B:210:VAL:HG13	5:B:211:HIS:H	1.79	0.47
7:D:21:LEU:HD22	7:D:37:VAL:HG11	1.97	0.47
8:E:11:ARG:NH1	8:E:20:LEU:HD22	2.30	0.47
8:E:105:VAL:HG12	8:E:244:ILE:N	2.30	0.47
10:G:67:VAL:HG12	10:G:69:LEU:H	1.80	0.47
10:G:148:THR:O	10:G:149:LYS:HB3	2.15	0.47
15:L:21:THR:HG23	15:L:32:LYS:HB2	1.97	0.47
25:V:11:LEU:O	25:V:12:TYR:CD2	2.68	0.47
44:p:483:VAL:HG21	44:p:538:TRP:HB2	1.97	0.47
44:p:688:GLU:HA	44:p:692:ALA:HB2	1.96	0.47
2:2:921:G:H2'	2:2:922:A:H8	1.80	0.46
2:2:1085:A:H5'	6:C:169:SER:HB3	1.97	0.46
3:A:195:TRP:CZ3	3:A:197:ILE:HD11	2.50	0.46
7:D:71:LEU:HD11	14:K:89:ALA:CB	2.37	0.46
20:Q:14:LYS:HB3	20:Q:15:SER:H	1.62	0.46
20:Q:130:GLY:HA2	20:Q:138:PHE:CE2	2.51	0.46
41:l:178:GLN:HB2	41:l:209:LYS:HA	1.96	0.46
2:2:568:C:H41	27:X:69:ARG:NH2	2.13	0.46
3:A:79:ARG:HD2	3:A:81:TYR:CD1	2.50	0.46
23:T:6:VAL:HG21	23:T:132:LEU:HD23	1.97	0.46
24:U:34:LEU:HD21	24:U:89:ARG:HG3	1.98	0.46
30:a:36:ILE:HD13	30:a:78:ALA:HB1	1.94	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:b:41:LEU:HD11	45:q:497:ALA:HB3	1.96	0.46
32:c:12:VAL:HG12	32:c:30:VAL:HA	1.96	0.46
36:g:143:TYR:CD2	36:g:193:TYR:CE1	3.03	0.46
38:i:56:LYS:C	38:i:56:LYS:CD	2.89	0.46
39:j:14:PRO:HG3	39:j:40:ASP:HB2	1.96	0.46
39:j:226:PRO:HA	40:k:405:THR:HG22	1.97	0.46
2:2:459:A:H3'	2:2:460:G:H8	1.80	0.46
2:2:1290:G:N2	2:2:1323:G:H22	2.09	0.46
30:a:59:TYR:HE1	30:a:62:TYR:CG	2.33	0.46
41:l:168:ASP:HB3	41:l:171:LYS:HB3	1.97	0.46
42:m:22:THR:C	42:m:24:ASN:H	2.24	0.46
42:m:94:SER:OG	42:m:95:GLN:N	2.48	0.46
44:p:316:ASP:HB3	44:p:321:LEU:H	1.80	0.46
44:p:628:SER:HB2	44:p:655:PHE:H	1.81	0.46
45:q:567:LEU:HD23	45:q:571:LEU:HD13	1.98	0.46
2:2:28:A:H2'	2:2:29:U:O4'	2.15	0.46
2:2:747:C:H42	2:2:801:G:H1	1.62	0.46
2:2:1458:A:C1'	19:P:129:GLY:HA3	2.46	0.46
6:C:234:LEU:HD21	25:V:13:VAL:HG13	1.97	0.46
11:H:162:ILE:CG2	11:H:166:LEU:CD2	2.89	0.46
21:R:113:LEU:O	21:R:115:LEU:N	2.48	0.46
36:g:50:GLU:HA	36:g:55:PHE:CD1	2.49	0.46
39:j:195:TYR:HE2	40:k:372:PRO:O	1.98	0.46
40:k:126:VAL:O	40:k:126:VAL:HG12	2.15	0.46
40:k:132:LEU:HD22	40:k:138:ILE:H	1.80	0.46
2:2:208:U:H2'	2:2:209:A:O4'	2.16	0.46
5:B:32:ILE:HB	5:B:43:VAL:HB	1.97	0.46
7:D:191:ASP:OD2	7:D:193:SER:OG	2.22	0.46
19:P:96:VAL:HB	19:P:103:ASN:HB2	1.97	0.46
30:a:82:ARG:HD2	30:a:85:ARG:HH22	1.81	0.46
36:g:84:ALA:HB1	36:g:111:VAL:HG12	1.98	0.46
36:g:143:TYR:HB2	36:g:193:TYR:CE1	2.51	0.46
44:p:560:PHE:CE2	44:p:642:ILE:HG22	2.51	0.46
2:2:679:U:H4'	2:2:680:U:OP2	2.15	0.46
2:2:1068:A:H2'	2:2:1069:C:O4'	2.15	0.46
2:2:1180:U:O2'	19:P:128:HIS:HE1	1.97	0.46
5:B:221:PRO:O	5:B:222:LYS:HB2	2.15	0.46
13:J:3:ARG:HD2	13:J:4:ALA:H	1.80	0.46
28:Y:5:ILE:CG2	28:Y:27:VAL:HG22	2.46	0.46
30:a:31:PRO:HG2	30:a:34:LYS:HB3	1.97	0.46
41:l:156:PRO:HG3	41:l:240:LYS:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:523:U:H2'	2:2:525:A:OP2	2.16	0.46
2:2:894:G:H22	2:2:916:U:H3	1.62	0.46
14:K:54:PHE:HE2	14:K:75:TYR:HB2	1.81	0.46
39:j:70:VAL:HG11	39:j:94:ASP:OD2	2.15	0.46
40:k:139:LYS:HD3	40:k:319:ARG:HD3	1.97	0.46
2:2:335:G:H1	12:I:5:ARG:HB3	1.80	0.46
2:2:1051:U:H3'	2:2:1052:G:C5'	2.45	0.46
2:2:1599:G:H22	23:T:88:VAL:HG22	1.80	0.46
2:2:1752:A:N3	38:i:44:ASN:ND2	2.59	0.46
3:A:170:ILE:HG12	3:A:171:GLY:N	2.30	0.46
7:D:144:ALA:O	7:D:146:ARG:N	2.49	0.46
11:H:44:LYS:O	11:H:44:LYS:HD3	2.15	0.46
11:H:93:LEU:HD22	11:H:125:ILE:HG23	1.97	0.46
14:K:50:THR:O	14:K:53:GLY:CA	2.64	0.46
21:R:20:TYR:CD1	21:R:23:LYS:HD2	2.50	0.46
23:T:35:ASP:N	23:T:54:PHE:CZ	2.81	0.46
24:U:63:LEU:HB3	33:d:34:TYR:OH	2.16	0.46
25:V:38:GLN:HB2	25:V:46:ILE:HB	1.98	0.46
28:Y:8:ARG:CZ	28:Y:28:LEU:HD11	2.45	0.46
30:a:36:ILE:CD1	30:a:78:ALA:HB2	2.10	0.46
39:j:23:ASN:HD21	39:j:66:GLY:HA2	1.81	0.46
40:k:128:PHE:CZ	40:k:132:LEU:HD11	2.24	0.46
44:p:364:ASN:OD1	44:p:365:PHE:N	2.40	0.46
44:p:421:GLU:HG2	44:p:422:VAL:N	2.31	0.46
2:2:1023:U:H2'	2:2:1024:A:H5''	1.98	0.46
2:2:1485:A:H2'	2:2:1486:G:H8	1.81	0.46
5:B:136:ARG:HH12	5:B:218:LEU:HD21	1.81	0.46
9:F:153:GLY:O	9:F:156:ALA:HB3	2.15	0.46
43:o:702:UNK:O	43:o:704:UNK:N	2.49	0.46
2:2:1232:G:H1	2:2:1251:C:H42	1.64	0.46
3:A:188:LEU:HD21	3:A:195:TRP:CD1	2.51	0.46
5:B:6:ASN:O	5:B:8:ARG:HG3	2.16	0.46
16:M:52:LEU:HB2	16:M:117:TRP:CZ3	2.51	0.46
22:S:28:VAL:HG11	22:S:47:CYS:SG	2.56	0.46
24:U:27:THR:HG22	24:U:88:LYS:HE2	1.98	0.46
36:g:47:ARG:CD	36:g:59:VAL:CG1	2.84	0.46
38:i:52:PHE:HB3	38:i:110:PRO:HD2	1.98	0.46
39:j:119:PHE:C	39:j:121:ILE:HD13	2.41	0.46
40:k:289:TYR:O	40:k:290:ASN:C	2.58	0.46
44:p:195:ASP:HB2	44:p:198:VAL:HA	1.98	0.46
44:p:491:GLU:HB3	44:p:504:ILE:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:773:C:OP2	8:E:23:LEU:HD23	2.16	0.45
3:A:81:TYR:HB3	3:A:167:LYS:CG	2.44	0.45
3:A:88:LYS:CD	3:A:202:TYR:CE1	2.74	0.45
7:D:219:GLU:CG	7:D:220:PRO:HD3	2.38	0.45
23:T:38:LYS:HD2	23:T:43:ASN:HB3	1.97	0.45
28:Y:92:VAL:HG11	28:Y:99:LYS:HE2	1.98	0.45
32:c:35:ASP:O	32:c:36:THR:OG1	2.29	0.45
42:m:69:VAL:HB	42:m:77:ILE:HB	1.98	0.45
43:o:264:PHE:HA	43:o:267:MET:HB2	1.98	0.45
44:p:504:ILE:HG21	44:p:550:ASN:HA	1.98	0.45
3:A:88:LYS:CG	3:A:202:TYR:CD1	2.81	0.45
8:E:161:LYS:HB3	8:E:171:ASP:H	1.81	0.45
8:E:238:LEU:CD1	8:E:242:LYS:HE3	2.46	0.45
14:K:87:PHE:HB3	14:K:91:TYR:CD1	2.52	0.45
21:R:116:LYS:O	21:R:117:LEU:HD23	2.17	0.45
40:k:136:ILE:HA	51:k:602:GCP:C3B	2.35	0.45
42:m:28:ILE:HD13	42:m:85:ARG:HB3	1.98	0.45
2:2:1745:G:H2'	2:2:1746:G:C8	2.51	0.45
24:U:39:ALA:O	24:U:42:ILE:HG22	2.16	0.45
29:Z:57:TYR:HD2	29:Z:59:TYR:O	1.92	0.45
30:a:10:ARG:O	30:a:11:ASN:CB	2.64	0.45
36:g:80:TYR:HE1	36:g:101:GLU:OE2	1.99	0.45
40:k:232:HIS:O	40:k:236:ILE:CG1	2.53	0.45
2:2:1351:U:H3	2:2:1371:A:H61	1.65	0.45
7:D:138:ILE:HB	7:D:150:MET:HB2	1.98	0.45
10:G:57:ASP:HA	10:G:106:LEU:HA	1.98	0.45
14:K:28:ASN:H	14:K:40:LEU:HD21	1.82	0.45
22:S:68:ARG:O	22:S:72:ILE:HG12	2.16	0.45
23:T:40:SER:HA	23:T:97:SER:HB3	1.98	0.45
26:W:76:SER:CB	26:W:77:PRO:CD	2.94	0.45
28:Y:57:VAL:HG12	28:Y:73:GLY:HA2	1.98	0.45
38:i:48:GLU:HG2	38:i:56:LYS:HE3	1.98	0.45
44:p:134:MET:HE2	44:p:138:LYS:HE3	1.97	0.45
2:2:565:C:H4'	34:e:8:LEU:HD11	1.98	0.45
2:2:693:U:C3'	2:2:694:U:H5''	2.46	0.45
2:2:1598:A:H2'	2:2:1598:A:N3	2.32	0.45
14:K:54:PHE:CZ	14:K:75:TYR:CE1	3.05	0.45
14:K:55:VAL:HG22	14:K:68:LEU:HD21	1.95	0.45
29:Z:86:GLU:HG2	29:Z:86:GLU:O	2.17	0.45
31:b:3:LEU:N	31:b:3:LEU:HD22	2.32	0.45
35:f:107:LYS:HZ3	35:f:115:ALA:C	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:k:127:ARG:O	40:k:133:GLU:OE2	2.34	0.45
2:2:310:U:P	27:X:24:TRP:HZ2	2.39	0.45
2:2:914:A:N3	2:2:914:A:H2'	2.32	0.45
2:2:1451:G:H1'	19:P:97:TYR:HE1	1.81	0.45
6:C:47:GLY:O	6:C:50:VAL:HG12	2.17	0.45
8:E:71:LYS:NZ	8:E:76:VAL:CG2	2.77	0.45
11:H:27:LEU:C	11:H:29:ASN:H	2.25	0.45
16:M:97:ILE:HG12	16:M:104:ARG:NH2	2.29	0.45
21:R:24:LEU:HD13	21:R:54:THR:CG2	2.47	0.45
22:S:26:ILE:CG2	22:S:30:TYR:HB2	2.39	0.45
29:Z:39:ALA:C	29:Z:40:VAL:CG2	2.89	0.45
40:k:124:GLN:HG2	40:k:125:THR:N	2.32	0.45
40:k:135:ASN:C	40:k:136:ILE:HG23	2.41	0.45
44:p:92:VAL:H	44:p:93:PRO:HD3	1.80	0.45
45:q:255:PHE:HB3	45:q:355:PRO:HB3	1.97	0.45
2:2:68:A:H4'	2:2:69:G:OP2	2.17	0.45
2:2:1665:A:H2'	2:2:1666:G:O4'	2.17	0.45
5:B:48:VAL:HG11	5:B:61:LEU:HG	1.98	0.45
6:C:85:VAL:HA	6:C:107:VAL:HG22	1.99	0.45
6:C:96:ARG:HD3	6:C:97:ALA:N	2.32	0.45
8:E:106:LYS:HA	8:E:245:LYS:HE2	1.99	0.45
11:H:97:ARG:HA	11:H:97:ARG:NE	2.31	0.45
16:M:101:GLY:O	16:M:102:ASN:CB	2.65	0.45
27:X:35:GLY:O	27:X:39:LYS:HG3	2.16	0.45
28:Y:5:ILE:HG22	28:Y:27:VAL:HG22	1.99	0.45
38:i:56:LYS:HD3	38:i:57:ARG:N	2.32	0.45
2:2:1500:G:N7	23:T:102:ARG:NH2	2.65	0.45
6:C:173:ARG:HG2	6:C:204:SER:HB3	1.98	0.45
11:H:98:ILE:HG21	11:H:118:LEU:HD23	1.96	0.45
14:K:54:PHE:HZ	14:K:75:TYR:CD1	2.32	0.45
20:Q:24:ALA:HB1	20:Q:62:ASN:HD22	1.81	0.45
31:b:21:LEU:HD23	31:b:26:GLN:HB3	1.97	0.45
35:f:118:ARG:HG2	35:f:118:ARG:O	2.16	0.45
2:2:95:G:H5'	8:E:8:HIS:HB2	1.99	0.45
2:2:609:G:H21	27:X:19:ARG:HH12	1.63	0.45
2:2:1294:G:H1	2:2:1301:U:H3	1.65	0.45
5:B:133:TYR:HA	5:B:221:PRO:HD3	1.98	0.45
5:B:192:VAL:HG23	43:o:18:LEU:HD23	1.99	0.45
27:X:69:ARG:NH1	27:X:117:ILE:HD11	2.31	0.45
36:g:82:VAL:CG1	36:g:114:VAL:CG2	2.77	0.45
40:k:127:ARG:HB2	40:k:133:GLU:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:p:567:VAL:HG23	44:p:571:MET:HB3	1.99	0.45
2:2:399:A:H5'	12:I:25:ARG:HA	1.97	0.45
2:2:993:G:H1	2:2:1009:C:H42	1.65	0.45
2:2:1163:G:H1	2:2:1579:C:H42	1.65	0.45
2:2:1745:G:H2'	2:2:1746:G:H8	1.82	0.45
29:Z:53:GLU:OE1	29:Z:68:ARG:NH1	2.50	0.45
40:k:252:ASP:HB2	40:k:287:LEU:HD12	1.99	0.45
41:l:139:PHE:CA	41:l:142:LEU:HD13	2.47	0.45
45:q:443:LYS:HE2	45:q:447:LEU:HD23	1.98	0.45
2:2:628:U:H2'	2:2:629:A:C8	2.51	0.44
2:2:1099:G:HO2'	26:W:76:SER:N	2.10	0.44
15:L:87:ARG:HA	15:L:104:HIS:CE1	2.53	0.44
22:S:89:GLN:O	22:S:97:ASP:HB3	2.15	0.44
24:U:47:THR:O	24:U:49:LYS:NZ	2.40	0.44
2:2:305:U:H2'	2:2:306:G:C8	2.52	0.44
8:E:44:LEU:C	8:E:45:ILE:HG13	2.41	0.44
22:S:91:ASP:OD2	22:S:108:LYS:HE3	2.16	0.44
24:U:103:ILE:O	24:U:106:ILE:HG13	2.17	0.44
31:b:59:CYS:SG	31:b:61:THR:CG2	3.06	0.44
36:g:151:TRP:CE3	36:g:179:MET:HE1	2.52	0.44
36:g:289:THR:H	36:g:292:GLN:HE21	1.64	0.44
40:k:238:ILE:HG12	40:k:514:TRP:CD2	2.52	0.44
43:o:98:ASP:HA	43:o:185:LYS:HE2	1.99	0.44
44:p:421:GLU:CD	44:p:424:ARG:HD2	2.43	0.44
44:p:472:ARG:HD2	44:p:479:PRO:HG2	1.99	0.44
2:2:1198:G:N3	2:2:1198:G:C2'	2.80	0.44
2:2:1591:A:H2'	2:2:1592:G:C8	2.53	0.44
17:N:115:LEU:HD13	17:N:115:LEU:C	2.42	0.44
38:i:45:GLY:HA3	38:i:61:ILE:HG22	1.98	0.44
43:o:240:ARG:HB3	43:o:263:VAL:HG22	1.99	0.44
44:p:227:SER:HA	44:p:231:TRP:CZ2	2.52	0.44
44:p:422:VAL:H	44:p:423:PRO:HD3	1.81	0.44
44:p:557:ALA:HB2	44:p:619:GLY:HA3	1.98	0.44
45:q:486:LEU:HG	45:q:489:ILE:HD12	1.98	0.44
45:q:710:LEU:HD23	45:q:713:LEU:HD13	1.99	0.44
2:2:568:C:H41	27:X:69:ARG:CZ	2.30	0.44
2:2:1228:G:N7	35:f:102:VAL:HG11	2.30	0.44
7:D:126:VAL:HG12	7:D:131:ALA:HB2	1.98	0.44
12:I:41:LYS:CG	12:I:60:ILE:HD12	2.46	0.44
16:M:28:SER:CB	16:M:34:LEU:CD1	2.93	0.44
20:Q:131:GLY:HA2	20:Q:138:PHE:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:58:GLY:HA2	27:X:70:LYS:HA	2.00	0.44
27:X:62:LYS:NZ	27:X:118:PRO:HB3	2.32	0.44
28:Y:15:ASN:HD21	28:Y:17:LEU:HB2	1.81	0.44
36:g:202:HIS:ND1	36:g:228:TYR:CE2	2.86	0.44
40:k:224:CYS:HB2	40:k:225:PRO:HD3	1.99	0.44
2:2:709:C:H2'	2:2:710:U:H4'	1.99	0.44
3:A:81:TYR:CG	3:A:167:LYS:HG3	2.48	0.44
6:C:162:LYS:HE2	6:C:175:ILE:HG23	1.99	0.44
17:N:65:VAL:HG12	17:N:66:ILE:HG13	1.98	0.44
33:d:22:ARG:NH2	33:d:36:LEU:HA	2.33	0.44
43:o:266:LEU:HG	43:o:269:ILE:HD12	1.99	0.44
44:p:118:GLU:HG3	44:p:121:GLY:HA2	1.99	0.44
44:p:473:LEU:HG	44:p:478:ILE:HG12	1.99	0.44
2:2:694:U:H5'	2:2:695:U:H2'	1.99	0.44
2:2:1125:G:H5'	37:h:11:ARG:HD2	1.99	0.44
2:2:1441:U:H4'	2:2:1442:A:H8	1.83	0.44
7:D:40:ARG:HA	24:U:110:PRO:HB3	2.00	0.44
9:F:156:ALA:HB3	9:F:158:ARG:HH12	1.83	0.44
40:k:219:ALA:HB3	40:k:222:GLU:HB2	1.98	0.44
40:k:473:ALA:O	40:k:474:ARG:HB2	2.17	0.44
44:p:697:THR:O	44:p:711:LYS:CB	2.66	0.44
2:2:108:A:H2'	2:2:109:G:C8	2.53	0.44
2:2:522:G:H21	2:2:528:A:H62	1.64	0.44
2:2:590:A:H2'	2:2:591:G:H8	1.81	0.44
2:2:1289:U:H2'	2:2:1290:G:C8	2.53	0.44
2:2:1387:C:C4'	21:R:48:ASN:HB3	2.48	0.44
8:E:238:LEU:CB	8:E:242:LYS:HD2	2.47	0.44
9:F:45:PHE:H	9:F:50:PHE:HB2	1.83	0.44
10:G:147:LEU:HD23	10:G:151:ASP:HB2	1.99	0.44
17:N:112:LYS:O	17:N:116:ILE:HG13	2.17	0.44
33:d:24:SER:O	33:d:26:SER:N	2.50	0.44
36:g:104:PHE:CD2	36:g:139:GLY:HA2	2.53	0.44
36:g:184:ARG:NH1	36:g:198:ASP:CG	2.75	0.44
40:k:236:ILE:O	40:k:241:LEU:HB2	2.18	0.44
44:p:79:ILE:HD11	44:p:130:GLU:CA	2.48	0.44
2:2:1478:G:H1	2:2:1525:C:H42	1.66	0.44
10:G:31:ARG:N	10:G:34:GLN:OE1	2.51	0.44
10:G:36:VAL:HB	10:G:50:PHE:HB2	2.00	0.44
12:I:23:LYS:HB2	12:I:24:LYS:H	1.65	0.44
13:J:113:VAL:O	13:J:117:GLY:CA	2.61	0.44
22:S:46:VAL:HG21	22:S:73:MET:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Y:4:ALA:C	28:Y:5:ILE:HD12	2.43	0.44
43:o:199:PHE:HB3	43:o:252:LEU:HD11	2.00	0.44
44:p:456:ARG:HH11	44:p:467:ASN:HD21	1.65	0.44
45:q:338:THR:HA	45:q:341:VAL:HG22	1.99	0.44
9:F:117:LYS:HA	9:F:120:LEU:HD12	2.00	0.44
9:F:153:GLY:C	9:F:156:ALA:H	2.25	0.44
10:G:68:LEU:O	10:G:68:LEU:HD23	2.17	0.44
11:H:44:LYS:O	11:H:45:SER:HB3	2.18	0.44
11:H:55:LYS:HE2	11:H:87:ASP:OD1	2.18	0.44
13:J:170:GLY:O	13:J:174:ARG:CD	2.61	0.44
17:N:94:LYS:O	17:N:98:VAL:HG23	2.18	0.44
20:Q:116:LEU:HB3	20:Q:117:LEU:H	1.40	0.44
25:V:46:ILE:HA	25:V:47:PRO:HD3	1.88	0.44
29:Z:51:MET:O	29:Z:55:PRO:HD3	2.18	0.44
29:Z:88:ILE:H	29:Z:88:ILE:CD1	2.31	0.44
38:i:100:ALA:HA	38:i:103:LEU:HD12	2.00	0.44
40:k:240:LYS:O	40:k:241:LEU:HG	2.18	0.44
2:2:1485:A:H2'	2:2:1486:G:C8	2.52	0.43
9:F:193:ALA:HB3	29:Z:98:GLN:HE22	1.82	0.43
12:I:36:THR:CB	12:I:96:LEU:HB3	2.48	0.43
17:N:52:VAL:HG22	17:N:55:ARG:HH12	1.84	0.43
22:S:76:PRO:HG3	22:S:99:HIS:HB2	2.00	0.43
23:T:34:VAL:CG1	23:T:54:PHE:CE2	3.00	0.43
24:U:46:GLU:O	24:U:49:LYS:HE3	2.18	0.43
30:a:23:CYS:SG	30:a:24:VAL:N	2.91	0.43
39:j:160:PRO:HG2	39:j:166:LEU:HD12	1.99	0.43
40:k:143:ALA:HA	40:k:383:GLU:OE1	2.18	0.43
1:1:27:C:H2'	1:1:28:A:H8	1.76	0.43
2:2:31:C:N4	2:2:594:G:H1	2.15	0.43
2:2:1140:G:H2'	2:2:1141:A:C8	2.53	0.43
5:B:205:PHE:CD2	5:B:206:PRO:HD2	2.53	0.43
7:D:200:LYS:H	7:D:200:LYS:NZ	2.16	0.43
8:E:116:ASP:HA	8:E:119:ALA:HB3	1.98	0.43
9:F:188:ASN:HD22	9:F:190:LYS:H	1.66	0.43
10:G:31:ARG:HH11	10:G:31:ARG:HG2	1.83	0.43
10:G:32:ILE:CA	10:G:52:ILE:HG23	2.42	0.43
14:K:54:PHE:CE2	14:K:75:TYR:CG	3.05	0.43
16:M:67:LEU:HD21	35:f:106:TYR:CD1	2.53	0.43
27:X:141:GLU:HB3	27:X:142:LYS:H	1.65	0.43
29:Z:62:VAL:HG12	29:Z:77:ARG:HG2	1.99	0.43
31:b:36:LYS:HE2	31:b:43:ILE:HG23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:d:21:CYS:SG	33:d:23:ILE:CG2	3.00	0.43
36:g:87:ASP:O	36:g:88:LYS:HB2	2.18	0.43
40:k:220:GLY:H	40:k:250:LYS:HB2	1.83	0.43
2:2:939:A:H2'	2:2:940:A:C8	2.53	0.43
2:2:1269:G:H1'	2:2:1445:C:C6	2.52	0.43
2:2:1340:A:H4'	36:g:91:ARG:NH2	2.34	0.43
2:2:1421:U:H2'	2:2:1422:A:O4'	2.18	0.43
8:E:73:ASP:CA	8:E:164:LEU:HD21	2.47	0.43
10:G:7:TYR:CD1	10:G:124:ILE:HG13	2.53	0.43
11:H:149:ILE:HG23	11:H:180:GLN:HB3	2.00	0.43
13:J:162:SER:O	13:J:163:PRO:O	2.35	0.43
14:K:85:HIS:C	14:K:86:ILE:HD12	2.44	0.43
15:L:54:ILE:HG23	15:L:54:ILE:O	2.18	0.43
21:R:113:LEU:C	21:R:115:LEU:N	2.77	0.43
24:U:22:ILE:CD1	24:U:100:VAL:CG1	2.73	0.43
32:c:13:ILE:O	32:c:14:LYS:HD2	2.18	0.43
39:j:16:ILE:HG23	39:j:75:ARG:O	2.18	0.43
40:k:431:GLU:HG2	40:k:482:MET:HE3	1.99	0.43
2:2:309:C:O3'	27:X:24:TRP:CZ2	2.68	0.43
2:2:369:A:H2'	2:2:370:G:O4'	2.17	0.43
2:2:1108:G:H2'	2:2:1109:G:C8	2.53	0.43
3:A:194:PRO:O	3:A:195:TRP:HB2	2.19	0.43
5:B:90:GLU:OE2	5:B:225:LEU:HG	2.18	0.43
6:C:148:TYR:OH	6:C:155:GLN:N	2.51	0.43
13:J:104:PHE:O	13:J:147:MET:HE1	2.18	0.43
20:Q:130:GLY:CA	20:Q:138:PHE:CE2	3.02	0.43
30:a:12:LYS:HZ1	30:a:16:GLY:C	2.26	0.43
35:f:105:TYR:HH	35:f:106:TYR:HH	1.61	0.43
36:g:50:GLU:CG	36:g:55:PHE:CE1	2.81	0.43
36:g:73:VAL:HG12	36:g:74:VAL:N	2.33	0.43
40:k:505:ILE:HB	40:k:510:ARG:HD2	2.00	0.43
45:q:783:GLU:O	45:q:783:GLU:HG2	2.17	0.43
3:A:3:LEU:HD12	3:A:7:PHE:HB3	2.00	0.43
3:A:78:SER:HB3	3:A:129:ASP:OD2	2.18	0.43
10:G:32:ILE:CG2	10:G:33:GLY:N	2.82	0.43
11:H:30:ASN:HD22	11:H:30:ASN:H	1.66	0.43
17:N:35:GLU:HA	17:N:38:ILE:HG12	2.01	0.43
20:Q:130:GLY:HA3	20:Q:137:ARG:HE	1.83	0.43
21:R:33:ARG:HB3	36:g:151:TRP:CH2	2.53	0.43
36:g:185:SER:OG	36:g:197:ALA:HB3	2.19	0.43
41:l:232:GLU:HB2	41:l:268:VAL:HG11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:m:93:ILE:HA	42:m:98:LEU:CB	2.47	0.43
44:p:217:MET:HB2	44:p:621:TYR:OH	2.17	0.43
44:p:403:LEU:O	44:p:420:ALA:N	2.47	0.43
45:q:408:ILE:H	45:q:408:ILE:HG13	1.69	0.43
2:2:608:U:H5	27:X:22:ASN:C	2.27	0.43
2:2:1600:C:H2'	2:2:1601:U:O4'	2.19	0.43
3:A:58:VAL:O	3:A:62:ARG:HG3	2.18	0.43
3:A:176:LEU:O	3:A:180:GLU:HG2	2.18	0.43
10:G:66:GLY:O	10:G:67:VAL:HB	2.18	0.43
11:H:8:ILE:HG13	11:H:9:LEU:HD12	2.01	0.43
22:S:28:VAL:HG12	22:S:29:VAL:HG23	2.00	0.43
22:S:119:ILE:O	22:S:120:ARG:HG2	2.18	0.43
26:W:3:ARG:CZ	26:W:28:ARG:CZ	2.96	0.43
40:k:217:LEU:HB3	40:k:249:ASN:HD22	1.83	0.43
40:k:238:ILE:CB	40:k:514:TRP:HB3	2.48	0.43
44:p:349:ALA:HB1	44:p:356:LEU:HD11	2.01	0.43
45:q:585:LEU:HD12	45:q:588:ILE:HD11	2.00	0.43
2:2:248:U:H3	15:L:17:PRO:HG2	1.84	0.43
2:2:608:U:C6	27:X:22:ASN:HB3	2.54	0.43
11:H:73:VAL:C	11:H:75:ILE:N	2.77	0.43
23:T:35:ASP:OD2	23:T:54:PHE:CE2	2.72	0.43
36:g:113:SER:HB3	36:g:126:ALA:HB3	2.00	0.43
40:k:355:ILE:HG21	40:k:415:GLN:HB3	1.99	0.43
44:p:179:ASP:C	44:p:181:PRO:HD3	2.43	0.43
45:q:263:ASP:OD1	45:q:357:GLU:OE2	2.36	0.43
2:2:394:U:O2'	10:G:89:ASN:HB3	2.18	0.43
3:A:41:ARG:HH11	3:A:43:ASP:CG	2.27	0.43
3:A:175:TYR:HD1	3:A:202:TYR:CE2	2.37	0.43
6:C:50:VAL:HG21	6:C:73:ILE:HG23	2.01	0.43
8:E:104:ASP:HB3	8:E:110:ALA:HB2	2.01	0.43
10:G:225:GLU:HB3	10:G:226:VAL:H	1.58	0.43
11:H:30:ASN:H	11:H:30:ASN:ND2	2.17	0.43
12:I:107:THR:N	12:I:108:PRO:HD2	2.33	0.43
15:L:87:ARG:CZ	15:L:104:HIS:CG	3.02	0.43
26:W:30:SER:CB	26:W:61:ILE:CD1	2.96	0.43
36:g:128:ARG:HG2	36:g:151:TRP:CG	2.54	0.43
36:g:153:THR:O	36:g:154:LYS:HG3	2.19	0.43
39:j:119:PHE:O	39:j:120:GLN:CB	2.66	0.43
44:p:218:PHE:O	44:p:219:ASN:C	2.62	0.43
45:q:373:VAL:HB	45:q:407:LEU:HD22	2.01	0.43
45:q:373:VAL:HG11	45:q:408:ILE:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1170:A:H2'	2:2:1171:G:H8	1.83	0.43
2:2:1675:C:H2'	2:2:1676:A:O4'	2.19	0.43
3:A:115:PHE:HZ	6:C:44:THR:HG22	1.84	0.43
5:B:143:THR:HG21	5:B:156:ALA:HB2	2.01	0.43
9:F:66:ILE:C	9:F:66:ILE:HD12	2.43	0.43
13:J:80:LEU:HA	13:J:83:ILE:HG22	2.00	0.43
16:M:17:ILE:HA	16:M:130:HIS:HD2	1.84	0.43
21:R:24:LEU:HD23	21:R:34:LEU:HD13	2.01	0.43
22:S:36:ARG:HB3	22:S:102:ALA:CB	2.49	0.43
25:V:25:LYS:HB2	25:V:28:ASP:HB2	2.01	0.43
27:X:79:ASN:HD22	27:X:81:LYS:H	1.66	0.43
36:g:11:ARG:HA	36:g:11:ARG:HE	1.83	0.43
36:g:113:SER:HB2	36:g:154:LYS:HA	2.01	0.43
36:g:156:ARG:HE	36:g:210:GLN:NE2	2.02	0.43
43:o:727:UNK:O	43:o:728:UNK:C	2.67	0.43
2:2:144:A:H61	2:2:168:A:H62	1.67	0.43
2:2:310:U:H5'	27:X:24:TRP:CH2	2.54	0.43
2:2:1091:A:O2'	2:2:1092:A:H2'	2.18	0.43
10:G:30:LYS:O	10:G:101:ILE:HA	2.18	0.43
22:S:103:ASN:O	22:S:103:ASN:ND2	2.50	0.43
40:k:128:PHE:H	40:k:132:LEU:HD12	1.84	0.43
40:k:217:LEU:HB3	40:k:249:ASN:HB2	2.01	0.43
1:1:28:A:H61	1:1:42:U:H3	1.66	0.42
2:2:626:C:H2'	2:2:627:G:O4'	2.19	0.42
2:2:710:U:H5'	2:2:711:G:C5	2.54	0.42
5:B:128:LYS:HG2	5:B:133:TYR:O	2.19	0.42
7:D:170:THR:HA	7:D:187:LYS:HG3	2.01	0.42
9:F:74:HIS:HB3	20:Q:47:LYS:HD2	2.00	0.42
11:H:141:ARG:HB3	26:W:51:GLU:HB3	2.00	0.42
39:j:40:ASP:CG	39:j:42:ILE:H	2.28	0.42
39:j:51:LEU:HG	39:j:87:LYS:HD2	2.00	0.42
40:k:211:MET:HB3	40:k:241:LEU:HD21	2.01	0.42
2:2:40:A:H2'	2:2:41:A:O4'	2.19	0.42
2:2:862:A:H62	2:2:963:U:H3	1.67	0.42
2:2:1391:C:H42	2:2:1403:G:H1	1.67	0.42
17:N:22:ALA:HB2	17:N:66:ILE:HG12	2.01	0.42
28:Y:29:HIS:ND1	28:Y:29:HIS:O	2.52	0.42
29:Z:86:GLU:HB3	29:Z:88:ILE:CD1	2.49	0.42
35:f:119:LYS:CE	35:f:120:GLU:CD	2.91	0.42
36:g:112:LEU:CD1	36:g:128:ARG:HG3	2.43	0.42
44:p:214:TRP:HE1	44:p:225:VAL:HB	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:p:359:HIS:CB	44:p:365:PHE:HD2	2.30	0.42
45:q:510:THR:O	45:q:514:LYS:CG	2.66	0.42
2:2:339:U:H2'	2:2:340:A:C8	2.54	0.42
2:2:357:U:H2'	2:2:359:A:H8	1.85	0.42
5:B:177:GLN:HE21	5:B:177:GLN:HB2	1.64	0.42
9:F:115:ILE:HG23	9:F:193:ALA:HB2	2.02	0.42
30:a:36:ILE:HB	30:a:73:TYR:HB3	1.93	0.42
33:d:23:ILE:CD1	33:d:46:LYS:HZ2	2.15	0.42
36:g:35:VAL:HG21	36:g:74:VAL:HG22	2.01	0.42
36:g:171:ARG:HA	36:g:189:ASN:OD1	2.19	0.42
36:g:196:GLU:O	36:g:235:LYS:HE2	2.19	0.42
40:k:493:THR:HG21	40:k:517:ILE:O	2.19	0.42
2:2:625:U:H2'	2:2:626:C:C6	2.54	0.42
2:2:625:U:H2'	2:2:626:C:H6	1.83	0.42
6:C:43:VAL:HG22	6:C:44:THR:N	2.35	0.42
7:D:200:LYS:H	7:D:200:LYS:CE	2.32	0.42
33:d:31:ILE:O	33:d:37:ASN:CA	2.62	0.42
35:f:117:LEU:O	35:f:118:ARG:HB3	2.19	0.42
2:2:898:G:H21	2:2:914:A:H2	1.67	0.42
11:H:70:TYR:O	11:H:74:GLN:HB2	2.18	0.42
36:g:107:HIS:CE1	36:g:133:ARG:HG3	2.55	0.42
36:g:258:TRP:CZ2	36:g:278:ILE:HD13	2.52	0.42
45:q:402:GLN:HG2	45:q:458:ILE:HD11	2.02	0.42
2:2:52:U:H2'	2:2:53:G:C8	2.54	0.42
6:C:58:ILE:H	6:C:58:ILE:HG13	1.46	0.42
9:F:45:PHE:HE1	9:F:117:LYS:NZ	2.09	0.42
10:G:31:ARG:O	10:G:32:ILE:CB	2.68	0.42
11:H:97:ARG:CG	11:H:99:LEU:HG	2.46	0.42
15:L:86:ILE:HB	15:L:107:VAL:HB	2.01	0.42
15:L:99:ARG:HG2	27:X:9:LEU:HD22	2.01	0.42
20:Q:131:GLY:CA	20:Q:138:PHE:CE1	3.03	0.42
22:S:26:ILE:HG22	22:S:27:ASN:N	2.35	0.42
28:Y:35:VAL:HG23	28:Y:36:SER:N	2.34	0.42
32:c:14:LYS:HB2	32:c:29:ARG:HD2	2.02	0.42
44:p:278:SER:HA	44:p:279:PRO:HD3	1.92	0.42
2:2:564:C:H4'	2:2:565:C:OP2	2.18	0.42
2:2:569:A:N6	27:X:69:ARG:NH1	2.66	0.42
2:2:813:A:N6	2:2:856:U:N3	2.62	0.42
2:2:1387:C:H4'	21:R:48:ASN:HB3	2.00	0.42
8:E:180:LEU:HD13	8:E:232:GLY:H	1.84	0.42
9:F:76:ALA:HB2	9:F:109:LYS:HZ3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:I:196:ARG:HD3	15:L:11:ARG:HH12	1.84	0.42
27:X:23:ARG:HB3	27:X:29:TYR:CD2	2.54	0.42
39:j:119:PHE:CB	39:j:121:ILE:CD1	2.88	0.42
43:o:706:UNK:O	43:o:710:UNK:N	2.53	0.42
44:p:159:THR:O	44:p:160:MET:CB	2.67	0.42
2:2:1540:G:H5''	23:T:87:GLY:C	2.44	0.42
2:2:1605:G:H2'	2:2:1606:U:C6	2.55	0.42
6:C:83:ASP:HA	6:C:109:VAL:HG23	2.01	0.42
8:E:18:TRP:HB3	8:E:20:LEU:HG	2.01	0.42
8:E:238:LEU:HD12	8:E:242:LYS:HE3	2.02	0.42
15:L:123:VAL:HG22	15:L:142:VAL:HA	2.00	0.42
24:U:47:THR:HA	24:U:49:LYS:HZ1	1.85	0.42
24:U:118:ILE:HD12	24:U:118:ILE:C	2.45	0.42
25:V:10:GLU:C	25:V:11:LEU:CG	2.81	0.42
25:V:12:TYR:HD1	25:V:13:VAL:C	2.27	0.42
29:Z:84:GLU:OE2	29:Z:89:ILE:CD1	2.62	0.42
44:p:311:GLN:H	44:p:327:PRO:HB3	1.85	0.42
2:2:410:C:H2'	2:2:411:A:O4'	2.20	0.42
2:2:1038:A:O2'	2:2:1039:G:H5''	2.20	0.42
3:A:88:LYS:HD2	3:A:201:LEU:HB3	2.02	0.42
5:B:130:SER:HB2	5:B:179:SER:O	2.20	0.42
7:D:144:ALA:C	7:D:146:ARG:N	2.77	0.42
9:F:65:GLN:C	9:F:66:ILE:HG13	2.44	0.42
14:K:9:LYS:HE3	14:K:80:LEU:HG	2.02	0.42
14:K:64:TYR:CB	14:K:66:TYR:HE2	2.24	0.42
14:K:87:PHE:HD2	14:K:91:TYR:CB	2.27	0.42
28:Y:29:HIS:CE1	28:Y:32:ARG:C	2.96	0.42
34:e:8:LEU:HD23	38:i:90:ASP:OD1	2.20	0.42
36:g:5:ASN:O	36:g:324:THR:HA	2.20	0.42
39:j:10:GLU:HG3	39:j:136:ARG:HD2	2.02	0.42
39:j:93:GLU:O	39:j:93:GLU:HG2	2.19	0.42
40:k:238:ILE:CD1	40:k:513:GLY:O	2.62	0.42
2:2:65:A:H2	2:2:84:A:H62	1.68	0.42
8:E:105:VAL:HG12	8:E:244:ILE:C	2.40	0.42
12:I:21:PHE:CD1	12:I:21:PHE:C	2.98	0.42
12:I:35:ASN:OD1	12:I:58:LEU:HD21	2.20	0.42
15:L:42:PHE:HE1	15:L:141:LYS:HB2	1.84	0.42
21:R:45:ARG:HG2	21:R:49:LYS:HE2	2.02	0.42
24:U:49:LYS:N	24:U:49:LYS:CD	2.80	0.42
31:b:55:THR:HG22	31:b:62:VAL:HA	2.01	0.42
45:q:354:GLU:HB3	45:q:355:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:1001:G:H4'	42:m:67:ASN:HD21	1.85	0.41
20:Q:131:GLY:N	20:Q:138:PHE:CZ	2.88	0.41
23:T:28:LEU:HB3	23:T:30:VAL:HG13	2.01	0.41
30:a:10:ARG:HG3	30:a:34:LYS:CE	2.50	0.41
31:b:54:VAL:HB	31:b:63:LEU:HD12	2.02	0.41
39:j:121:ILE:N	39:j:121:ILE:CD1	2.75	0.41
45:q:115:ALA:O	45:q:116:LYS:C	2.64	0.41
2:2:1287:G:H1	2:2:1326:C:H42	1.69	0.41
9:F:65:GLN:C	9:F:67:SER:N	2.77	0.41
20:Q:49:TYR:HA	20:Q:52:LEU:HD12	2.02	0.41
25:V:8:LEU:CD2	25:V:10:GLU:HB3	2.51	0.41
25:V:11:LEU:O	25:V:12:TYR:CG	2.73	0.41
27:X:92:CYS:SG	27:X:135:LEU:HB3	2.60	0.41
28:Y:5:ILE:CD1	28:Y:5:ILE:N	2.82	0.41
28:Y:54:ALA:HB1	28:Y:76:TYR:HB2	2.03	0.41
39:j:56:ILE:HG13	39:j:56:ILE:O	2.21	0.41
2:2:454:C:H3'	2:2:455:A:H8	1.85	0.41
2:2:594:G:H2'	2:2:595:C:C6	2.55	0.41
2:2:654:G:H2'	2:2:655:G:C8	2.54	0.41
2:2:862:A:H2'	2:2:864:A:C8	2.55	0.41
2:2:887:U:H2'	2:2:888:U:C6	2.55	0.41
2:2:1391:C:H4'	36:g:288:TYR:CE2	2.55	0.41
2:2:1607:U:H2'	2:2:1608:G:O4'	2.20	0.41
5:B:24:PHE:CD2	5:B:27:LYS:HE3	2.55	0.41
6:C:61:ILE:O	6:C:65:SER:N	2.52	0.41
6:C:153:LEU:HD12	6:C:153:LEU:HA	1.90	0.41
13:J:105:LEU:O	13:J:108:ARG:HB2	2.19	0.41
13:J:120:LYS:O	13:J:121:SER:OG	2.27	0.41
16:M:59:VAL:HG23	16:M:62:GLU:H	1.84	0.41
22:S:103:ASN:ND2	22:S:103:ASN:C	2.78	0.41
24:U:68:ARG:HD3	24:U:79:TRP:CE2	2.56	0.41
26:W:3:ARG:NH2	26:W:28:ARG:NH1	2.67	0.41
36:g:29:ALA:CB	36:g:77:ASP:CA	2.91	0.41
40:k:233:LEU:O	40:k:236:ILE:HB	2.20	0.41
43:o:721:UNK:CB	44:p:194:MET:CB	2.98	0.41
2:2:568:C:H41	27:X:69:ARG:NH1	2.18	0.41
2:2:1612:A:H5'	2:2:1613:C:OP2	2.20	0.41
2:2:1682:U:H2'	2:2:1683:G:H8	1.85	0.41
8:E:136:ILE:HD13	8:E:148:ARG:HH12	1.85	0.41
13:J:3:ARG:HD2	13:J:4:ALA:N	2.34	0.41
13:J:49:LEU:CD2	13:J:100:LYS:O	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:K:54:PHE:HE2	14:K:75:TYR:CG	2.38	0.41
17:N:109:LYS:H	17:N:109:LYS:HG3	1.67	0.41
27:X:92:CYS:HA	27:X:95:PHE:HD1	0.61	0.41
29:Z:57:TYR:CE2	29:Z:59:TYR:N	2.88	0.41
40:k:130:ASP:OD1	40:k:134:ARG:CD	2.62	0.41
44:p:522:ARG:HB3	44:p:543:GLU:HG3	2.03	0.41
2:2:589:C:H2'	2:2:590:A:C8	2.55	0.41
3:A:98:ILE:HD13	3:A:102:PHE:CE2	2.56	0.41
5:B:176:VAL:HA	5:B:184:LEU:HD21	2.02	0.41
6:C:157:HIS:CD2	6:C:200:ASP:OD2	2.73	0.41
8:E:238:LEU:CD1	8:E:242:LYS:CE	2.99	0.41
28:Y:31:ASN:ND2	28:Y:31:ASN:C	2.79	0.41
28:Y:128:LYS:HG3	28:Y:131:ARG:HH22	1.86	0.41
39:j:226:PRO:CA	40:k:405:THR:HG22	2.50	0.41
40:k:376:ASN:HD22	40:k:401:LYS:HE3	1.85	0.41
42:m:42:VAL:HB	42:m:78:ILE:HB	2.02	0.41
2:2:747:C:H2'	2:2:748:U:O4'	2.21	0.41
2:2:989:C:H2'	2:2:990:G:C8	2.55	0.41
2:2:1135:U:H2'	2:2:1136:A:C8	2.56	0.41
2:2:1741:U:H2'	2:2:1742:A:H5''	2.01	0.41
9:F:99:LEU:HD22	9:F:112:ALA:HA	2.03	0.41
9:F:189:ILE:HD13	29:Z:66:VAL:HG11	2.02	0.41
11:H:165:LYS:O	11:H:169:PHE:HB2	2.21	0.41
12:I:153:ILE:O	12:I:154:GLU:HB3	2.20	0.41
23:T:70:GLN:HA	23:T:122:ARG:H	1.86	0.41
25:V:79:LEU:HD22	25:V:82:VAL:HG21	2.02	0.41
27:X:135:LEU:HD23	27:X:141:GLU:HG3	2.03	0.41
28:Y:28:LEU:N	28:Y:28:LEU:CD1	2.83	0.41
37:h:8:LYS:HD3	37:h:12:ARG:HH12	1.85	0.41
39:j:48:LEU:CD2	39:j:56:ILE:HD11	2.44	0.41
40:k:143:ALA:HA	40:k:383:GLU:CD	2.46	0.41
44:p:102:LEU:HD21	44:p:149:LEU:HD11	2.03	0.41
44:p:141:ILE:H	44:p:141:ILE:HG13	1.64	0.41
45:q:510:THR:CG2	45:q:514:LYS:CD	2.91	0.41
2:2:74:U:H4'	2:2:75:U:OP1	2.21	0.41
2:2:1331:C:OP1	21:R:43:SER:HB2	2.19	0.41
2:2:1710:A:H2'	2:2:1711:G:H4'	2.01	0.41
6:C:234:LEU:HD22	6:C:234:LEU:HA	1.85	0.41
7:D:119:ALA:O	7:D:122:VAL:HG12	2.20	0.41
9:F:185:ALA:HB2	9:F:192:ILE:HG12	2.02	0.41
16:M:52:LEU:HD13	16:M:52:LEU:C	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:93:LYS:O	17:N:96:VAL:HG12	2.21	0.41
22:S:11:PHE:CG	22:S:57:ARG:HD3	2.56	0.41
26:W:27:ILE:HG22	26:W:29:PRO:O	2.20	0.41
36:g:11:ARG:HA	36:g:11:ARG:NE	2.36	0.41
41:l:195:LEU:HA	41:l:198:GLU:HB2	2.02	0.41
45:q:396:ILE:H	45:q:396:ILE:HG13	1.72	0.41
2:2:512:U:C1'	13:J:131:GLN:HG3	2.47	0.41
3:A:124:THR:HA	3:A:146:LEU:HD13	2.03	0.41
9:F:65:GLN:HB3	9:F:91:ILE:HG13	2.01	0.41
10:G:109:LEU:HD12	10:G:111:LEU:HD11	2.03	0.41
15:L:142:VAL:HG12	15:L:145:ALA:H	1.86	0.41
18:O:25:ASP:OD1	18:O:26:THR:N	2.53	0.41
36:g:72:VAL:CG1	36:g:73:VAL:N	2.83	0.41
39:j:115:CYS:HA	39:j:118:LYS:HE2	2.02	0.41
43:o:180:SER:O	43:o:184:LYS:HB2	2.19	0.41
44:p:246:PHE:HE1	44:p:284:LEU:HD11	1.84	0.41
2:2:3:U:C6	6:C:184:VAL:HG13	2.56	0.41
2:2:123:G:H4'	8:E:145:ARG:HD2	2.03	0.41
2:2:363:G:O2'	2:2:757:A:N6	2.54	0.41
2:2:462:U:H2'	2:2:463:A:C8	2.56	0.41
2:2:1037:U:O4	2:2:1091:A:N1	2.54	0.41
2:2:1139:G:H2'	2:2:1140:G:C8	2.55	0.41
2:2:1300:U:H2'	2:2:1301:U:O4'	2.21	0.41
2:2:1391:C:H5''	36:g:292:GLN:OE1	2.21	0.41
2:2:1757:C:H2'	2:2:1758:G:O4'	2.20	0.41
5:B:7:LYS:C	5:B:8:ARG:HG3	2.45	0.41
5:B:90:GLU:CD	5:B:225:LEU:HG	2.46	0.41
6:C:118:LEU:HD11	6:C:216:LEU:HB3	2.03	0.41
7:D:50:ILE:HD11	7:D:86:LEU:HD22	2.03	0.41
14:K:89:ALA:C	14:K:91:TYR:H	2.28	0.41
15:L:111:VAL:HG13	15:L:139:VAL:HG21	2.02	0.41
18:O:56:SER:HA	18:O:57:PRO:HD3	1.96	0.41
18:O:89:THR:O	18:O:128:LYS:CE	2.65	0.41
20:Q:125:GLU:HA	20:Q:126:PRO:HD3	1.97	0.41
21:R:41:ILE:HD13	21:R:47:ARG:CG	2.51	0.41
22:S:76:PRO:HA	22:S:81:ILE:HD12	2.02	0.41
22:S:89:GLN:O	22:S:97:ASP:HA	2.21	0.41
27:X:103:LEU:HD12	27:X:125:VAL:HB	2.01	0.41
30:a:10:ARG:HA	30:a:34:LYS:HB2	2.02	0.41
36:g:274:ASN:O	36:g:276:VAL:HG23	2.21	0.41
39:j:197:GLY:C	39:j:198:ILE:HD12	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:k:238:ILE:HD13	40:k:513:GLY:C	2.45	0.41
43:o:430:ARG:HA	43:o:433:PHE:HD2	1.86	0.41
2:2:602:U:H2'	2:2:603:A:H8	1.86	0.41
8:E:43:PRO:HB2	8:E:45:ILE:HD12	2.01	0.41
9:F:92:VAL:HA	9:F:95:LEU:HD12	2.02	0.41
10:G:123:GLY:C	10:G:127:ASP:H	2.27	0.41
12:I:21:PHE:CD1	12:I:22:ARG:HB3	2.56	0.41
12:I:35:ASN:HB2	12:I:95:THR:HG22	2.03	0.41
28:Y:45:ALA:HA	28:Y:50:ALA:O	2.21	0.41
36:g:184:ARG:HB3	36:g:195:ILE:CD1	2.51	0.41
38:i:35:TYR:HB3	38:i:52:PHE:CD2	2.56	0.41
40:k:245:ILE:HG23	40:k:278:ALA:HB1	2.03	0.41
2:2:759:U:H2'	2:2:760:A:C8	2.56	0.40
2:2:1065:C:H4'	5:B:149:GLN:HG2	2.03	0.40
7:D:13:ALA:O	7:D:16:VAL:HG12	2.21	0.40
16:M:81:LYS:O	16:M:131:PHE:CZ	2.74	0.40
23:T:47:PRO:CB	23:T:53:TRP:CG	2.95	0.40
23:T:71:VAL:H	23:T:122:ARG:H	1.67	0.40
36:g:183:VAL:HB	36:g:199:PHE:HB2	2.03	0.40
43:o:8:PRO:HA	43:o:11:ALA:HB2	2.03	0.40
44:p:536:LYS:HG2	44:p:537:ARG:HG3	2.04	0.40
2:2:120:U:H2'	2:2:121:U:H6	1.86	0.40
2:2:330:A:H5''	12:I:56:ARG:NH2	2.36	0.40
2:2:371:G:H2'	2:2:372:G:O4'	2.21	0.40
2:2:813:A:N1	2:2:856:U:O4	2.54	0.40
2:2:994:A:H61	2:2:1008:U:H3	1.68	0.40
2:2:1331:C:O2'	7:D:162:GLN:HB2	2.21	0.40
23:T:105:LEU:HA	23:T:108:LEU:HD12	2.02	0.40
29:Z:84:GLU:CG	29:Z:89:ILE:HB	2.46	0.40
35:f:103:LEU:O	35:f:104:ASN:HB3	2.21	0.40
36:g:90:LEU:HB2	36:g:104:PHE:HB2	2.02	0.40
36:g:205:TYR:O	36:g:222:GLY:HA3	2.22	0.40
36:g:268:LYS:HE3	36:g:280:GLU:OE2	2.20	0.40
41:l:177:ILE:HG21	41:l:211:LEU:HB2	2.03	0.40
43:o:69:LYS:HG2	43:o:164:ALA:HB2	2.03	0.40
2:2:52:U:H2'	2:2:53:G:H8	1.86	0.40
2:2:514:A:H62	2:2:536:G:H21	1.68	0.40
2:2:645:U:H2'	2:2:646:G:H8	1.85	0.40
2:2:1180:U:H2'	2:2:1181:U:O4'	2.21	0.40
6:C:96:ARG:HB3	6:C:97:ALA:H	1.69	0.40
8:E:212:ASP:OD1	8:E:216:ASN:N	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:127:THR:O	9:F:127:THR:HG22	2.20	0.40
11:H:64:VAL:HG22	11:H:94:ALA:HB1	2.02	0.40
13:J:172:VAL:O	13:J:176:ARG:HG2	2.21	0.40
22:S:28:VAL:O	22:S:29:VAL:CB	2.68	0.40
23:T:80:TYR:HB2	23:T:96:ALA:HB2	2.03	0.40
26:W:35:ILE:HA	26:W:38:LEU:HD12	2.03	0.40
36:g:19:GLY:O	36:g:20:TRP:C	2.63	0.40
41:l:161:PRO:HG3	41:l:183:LYS:HD2	2.02	0.40
43:o:346:ASP:HA	43:o:347:PRO:HD3	1.90	0.40
1:1:43:G:H2'	1:1:44:A:C8	2.56	0.40
2:2:544:A:H61	2:2:592:U:H2'	1.86	0.40
3:A:67:ILE:HA	3:A:68:PRO:HD3	1.94	0.40
10:G:151:ASP:O	10:G:152:ASP:CB	2.68	0.40
11:H:97:ARG:NE	11:H:97:ARG:CA	2.84	0.40
22:S:18:LEU:HD23	22:S:19:ASN:N	2.30	0.40
40:k:503:ARG:HD3	40:k:512:ILE:HG21	2.02	0.40
44:p:412:ASN:C	44:p:412:ASN:ND2	2.78	0.40
2:2:954:A:H5''	17:N:10:GLY:HA3	2.02	0.40
2:2:1466:U:H5''	23:T:91:HIS:CE1	2.57	0.40
2:2:1671:G:OP1	10:G:94:ARG:NH2	2.54	0.40
13:J:4:ALA:HA	13:J:5:PRO:HD3	1.99	0.40
14:K:77:ARG:HA	14:K:82:LEU:HD23	2.04	0.40
14:K:86:ILE:CG2	14:K:87:PHE:N	2.83	0.40
15:L:94:VAL:HA	15:L:95:PRO:HD3	1.93	0.40
20:Q:137:ARG:HG3	20:Q:138:PHE:H	1.86	0.40
28:Y:12:VAL:HG13	28:Y:23:PHE:HB3	2.04	0.40
33:d:23:ILE:CD1	33:d:46:LYS:NZ	2.57	0.40
36:g:129:ASP:O	36:g:130:LYS:HB2	2.21	0.40
36:g:172:ILE:CG2	36:g:174:PHE:CZ	2.99	0.40
36:g:208:VAL:HG22	36:g:209:VAL:N	2.37	0.40
44:p:355:SER:HA	44:p:377:GLY:HA2	2.04	0.40
44:p:509:VAL:CG1	44:p:510:ALA:N	2.80	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	206/208 (99%)	185 (90%)	16 (8%)	5 (2%)	4	26
5	B	218/231 (94%)	190 (87%)	20 (9%)	8 (4%)	2	19
6	C	215/217 (99%)	196 (91%)	12 (6%)	7 (3%)	3	20
7	D	221/223 (99%)	193 (87%)	19 (9%)	9 (4%)	2	17
8	E	258/260 (99%)	231 (90%)	26 (10%)	1 (0%)	30	66
9	F	204/206 (99%)	182 (89%)	17 (8%)	5 (2%)	4	25
10	G	224/226 (99%)	204 (91%)	19 (8%)	1 (0%)	30	66
11	H	182/184 (99%)	158 (87%)	16 (9%)	8 (4%)	2	16
12	I	184/200 (92%)	165 (90%)	16 (9%)	3 (2%)	7	36
13	J	180/182 (99%)	161 (89%)	12 (7%)	7 (4%)	2	18
14	K	94/96 (98%)	82 (87%)	9 (10%)	3 (3%)	3	20
15	L	153/155 (99%)	140 (92%)	13 (8%)	0	100	100
16	M	113/118 (96%)	88 (78%)	22 (20%)	3 (3%)	4	24
17	N	148/150 (99%)	142 (96%)	6 (4%)	0	100	100
18	O	125/127 (98%)	112 (90%)	11 (9%)	2 (2%)	7	36
19	P	117/119 (98%)	86 (74%)	24 (20%)	7 (6%)	1	12
20	Q	139/141 (99%)	120 (86%)	16 (12%)	3 (2%)	5	27
21	R	105/125 (84%)	87 (83%)	11 (10%)	7 (7%)	1	11
22	S	143/145 (99%)	125 (87%)	16 (11%)	2 (1%)	9	38
23	T	141/143 (99%)	131 (93%)	8 (6%)	2 (1%)	9	38
24	U	104/106 (98%)	94 (90%)	9 (9%)	1 (1%)	12	47
25	V	85/87 (98%)	76 (89%)	8 (9%)	1 (1%)	10	42
26	W	127/129 (98%)	115 (91%)	9 (7%)	3 (2%)	4	26
27	X	142/144 (99%)	124 (87%)	13 (9%)	5 (4%)	3	20
28	Y	132/134 (98%)	118 (89%)	11 (8%)	3 (2%)	5	27
29	Z	68/70 (97%)	62 (91%)	5 (7%)	1 (2%)	8	38
30	a	96/98 (98%)	82 (85%)	11 (12%)	3 (3%)	3	21
31	b	79/81 (98%)	71 (90%)	8 (10%)	0	100	100
32	c	60/62 (97%)	54 (90%)	6 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	d	51/53 (96%)	41 (80%)	9 (18%)	1 (2%)	6	30
34	e	56/58 (97%)	45 (80%)	10 (18%)	1 (2%)	6	32
35	f	67/69 (97%)	46 (69%)	17 (25%)	4 (6%)	1	12
36	g	305/324 (94%)	289 (95%)	16 (5%)	0	100	100
37	h	23/25 (92%)	20 (87%)	3 (13%)	0	100	100
38	i	93/95 (98%)	87 (94%)	5 (5%)	1 (1%)	11	45
39	j	243/263 (92%)	207 (85%)	32 (13%)	4 (2%)	7	36
40	k	406/430 (94%)	345 (85%)	52 (13%)	9 (2%)	5	27
41	l	122/144 (85%)	100 (82%)	20 (16%)	2 (2%)	7	36
42	m	94/96 (98%)	74 (79%)	16 (17%)	4 (4%)	2	16
43	o	445/567 (78%)	371 (83%)	68 (15%)	6 (1%)	9	40
44	p	643/651 (99%)	537 (84%)	86 (13%)	20 (3%)	3	21
45	q	657/665 (99%)	537 (82%)	98 (15%)	22 (3%)	3	20
46	s	326/342 (95%)	318 (98%)	8 (2%)	0	100	100
47	r	47/49 (96%)	45 (96%)	2 (4%)	0	100	100
All	All	7841/8198 (96%)	6836 (87%)	831 (11%)	174 (2%)	7	27

All (174) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	B	26	ARG
5	B	210	VAL
6	C	235	TRP
7	D	195	ASN
9	F	46	ASN
10	G	32	ILE
11	H	64	VAL
11	H	74	GLN
11	H	87	ASP
12	I	153	ILE
16	M	102	ASN
16	M	111	VAL
18	O	93	THR
20	Q	32	ASN
20	Q	39	VAL
22	S	29	VAL
23	T	50	SER

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Mol	Chain	Res	Type
26	W	76	SER
27	X	3	LYS
29	Z	40	VAL
35	f	102	VAL
35	f	104	ASN
39	j	225	ALA
40	k	136	ILE
40	k	240	LYS
40	k	290	ASN
40	k	324	ASN
42	m	23	SER
42	m	75	GLY
42	m	94	SER
42	m	96	LEU
44	p	160	MET
44	p	736	GLN
45	q	357	GLU
5	B	207	LEU
5	B	221	PRO
6	C	43	VAL
7	D	130	GLY
7	D	145	ALA
9	F	65	GLN
9	F	100	MET
11	H	28	GLU
13	J	121	SER
13	J	163	PRO
13	J	182	GLY
19	P	109	PRO
21	R	76	GLU
21	R	98	ASP
35	f	84	VAL
38	i	22	PRO
39	j	198	ILE
44	p	185	PRO
44	p	411	ASN
44	p	529	LYS
45	q	336	ILE
45	q	460	PRO
45	q	652	ILE
3	A	5	SER
3	A	195	TRP

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Mol	Chain	Res	Type
6	C	79	PRO
6	C	240	LEU
7	D	5	ILE
9	F	102	ASN
13	J	35	GLY
16	M	32	ASP
19	P	108	ARG
21	R	22	PRO
21	R	23	LYS
21	R	114	GLY
25	V	12	TYR
26	W	57	ARG
28	Y	64	TYR
30	a	61	GLU
30	a	64	LEU
33	d	25	GLY
35	f	93	HIS
40	k	255	ARG
41	l	129	LEU
43	o	194	GLN
43	o	461	SER
44	p	125	GLY
45	q	114	SER
45	q	337	ASP
45	q	346	ASP
45	q	527	GLN
3	A	109	ASN
5	B	132	ASP
8	E	107	GLY
11	H	14	THR
11	H	45	SER
11	H	54	GLY
18	O	96	PRO
19	P	48	GLY
21	R	25	THR
21	R	115	LEU
23	T	96	ALA
24	U	19	ILE
26	W	58	SER
27	X	64	PRO
30	a	28	ARG
34	e	13	LYS

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Mol	Chain	Res	Type
39	j	75	ARG
40	k	278	ALA
40	k	495	ILE
41	l	188	PRO
43	o	392	GLU
43	o	487	ALA
44	p	180	MET
44	p	181	PRO
44	p	342	SER
44	p	364	ASN
45	q	341	VAL
45	q	468	THR
45	q	536	ASP
45	q	645	ILE
3	A	158	VAL
5	B	56	ASN
5	B	148	ASN
5	B	224	ASP
11	H	13	PRO
13	J	18	PRO
13	J	134	ILE
14	K	30	PRO
20	Q	34	SER
27	X	63	GLN
28	Y	36	SER
40	k	168	LYS
43	o	294	GLY
44	p	184	VAL
44	p	375	PRO
44	p	531	LYS
44	p	633	VAL
44	p	735	VAL
45	q	347	PRO
45	q	351	ILE
45	q	446	ASN
45	q	630	ILE
45	q	762	GLU
45	q	766	PRO
45	q	781	GLY
6	C	66	LEU
6	C	154	GLY
7	D	217	VAL

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Mol	Chain	Res	Type
9	F	66	ILE
14	K	93	ALA
19	P	75	VAL
27	X	89	ASN
13	J	165	GLY
14	K	88	PRO
40	k	393	GLY
44	p	121	GLY
44	p	422	VAL
44	p	509	VAL
45	q	205	VAL
7	D	216	PRO
12	I	80	GLY
19	P	99	GLY
19	P	129	GLY
22	S	76	PRO
7	D	4	ILE
12	I	122	GLY
19	P	87	PRO
28	Y	29	HIS
39	j	133	PRO
43	o	49	GLU
44	p	392	PRO
45	q	649	PRO
6	C	67	PRO
7	D	63	GLY
7	D	211	PRO
44	p	636	GLY
45	q	355	PRO
3	A	68	PRO
27	X	41	SER

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	174/176 (99%)	148 (85%)	26 (15%)	3	13
5	B	198/210 (94%)	170 (86%)	28 (14%)	3	14
6	C	176/176 (100%)	151 (86%)	25 (14%)	3	14
7	D	185/185 (100%)	152 (82%)	33 (18%)	2	10
8	E	223/223 (100%)	187 (84%)	36 (16%)	2	12
9	F	174/174 (100%)	142 (82%)	32 (18%)	1	9
10	G	192/192 (100%)	165 (86%)	27 (14%)	3	14
11	H	164/164 (100%)	132 (80%)	32 (20%)	1	8
12	I	147/158 (93%)	134 (91%)	13 (9%)	9	29
13	J	153/153 (100%)	132 (86%)	21 (14%)	3	14
14	K	88/88 (100%)	76 (86%)	12 (14%)	3	15
15	L	136/136 (100%)	123 (90%)	13 (10%)	8	25
16	M	93/94 (99%)	85 (91%)	8 (9%)	10	29
17	N	127/127 (100%)	111 (87%)	16 (13%)	4	17
18	O	96/96 (100%)	86 (90%)	10 (10%)	7	22
19	P	101/101 (100%)	90 (89%)	11 (11%)	6	21
20	Q	117/117 (100%)	101 (86%)	16 (14%)	3	14
21	R	102/113 (90%)	91 (89%)	11 (11%)	6	21
22	S	128/128 (100%)	113 (88%)	15 (12%)	5	19
23	T	117/117 (100%)	106 (91%)	11 (9%)	8	26
24	U	96/96 (100%)	91 (95%)	5 (5%)	21	42
25	V	73/73 (100%)	64 (88%)	9 (12%)	4	17
26	W	110/110 (100%)	98 (89%)	12 (11%)	6	21
27	X	119/119 (100%)	105 (88%)	14 (12%)	5	18
28	Y	108/108 (100%)	94 (87%)	14 (13%)	4	16
29	Z	60/60 (100%)	58 (97%)	2 (3%)	33	55
30	a	83/83 (100%)	79 (95%)	4 (5%)	23	44
31	b	71/71 (100%)	63 (89%)	8 (11%)	5	20
32	c	54/54 (100%)	50 (93%)	4 (7%)	13	33
33	d	46/46 (100%)	46 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	e	51/51 (100%)	46 (90%)	5 (10%)	7	24
35	f	58/60 (97%)	52 (90%)	6 (10%)	7	23
36	g	257/270 (95%)	255 (99%)	2 (1%)	73	78
37	h	23/23 (100%)	21 (91%)	2 (9%)	9	29
38	i	81/81 (100%)	71 (88%)	10 (12%)	4	17
39	j	224/237 (94%)	200 (89%)	24 (11%)	6	21
40	k	332/364 (91%)	311 (94%)	21 (6%)	16	37
41	l	120/132 (91%)	110 (92%)	10 (8%)	10	30
42	m	76/84 (90%)	68 (90%)	8 (10%)	6	22
43	o	404/438 (92%)	359 (89%)	45 (11%)	6	20
44	p	533/584 (91%)	486 (91%)	47 (9%)	9	29
45	q	509/615 (83%)	445 (87%)	64 (13%)	4	17
46	s	287/297 (97%)	286 (100%)	1 (0%)	86	84
47	r	40/40 (100%)	40 (100%)	0	100	100
All	All	6706/7024 (96%)	5993 (89%)	713 (11%)	9	22

All (713) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	6	THR
3	A	13	ASP
3	A	16	LEU
3	A	43	ASP
3	A	45	VAL
3	A	50	VAL
3	A	56	LYS
3	A	58	VAL
3	A	59	LEU
3	A	83	GLN
3	A	87	LEU
3	A	88	LYS
3	A	93	THR
3	A	101	ARG
3	A	108	THR
3	A	112	THR
3	A	113	ARG
3	A	148	ASP

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Mol	Chain	Res	Type
3	A	154	GLU
3	A	165	ARG
3	A	170	ILE
3	A	172	LEU
3	A	193	GLN
3	A	195	TRP
3	A	198	MET
3	A	201	LEU
5	B	20	VAL
5	B	29	TRP
5	B	32	ILE
5	B	39	GLU
5	B	52	VAL
5	B	59	ASP
5	B	65	VAL
5	B	68	VAL
5	B	73	LEU
5	B	78	ASP
5	B	105	PHE
5	B	109	LYS
5	B	110	LEU
5	B	125	VAL
5	B	130	SER
5	B	134	VAL
5	B	171	ILE
5	B	177	GLN
5	B	178	ASN
5	B	184	LEU
5	B	205	PHE
5	B	207	LEU
5	B	208	GLN
5	B	210	VAL
5	B	222	LYS
5	B	225	LEU
5	B	228	LEU
5	B	231	LEU
6	C	49	LEU
6	C	50	VAL
6	C	58	ILE
6	C	65	SER
6	C	81	LEU
6	C	84	GLU

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Mol	Chain	Res	Type
6	C	88	ILE
6	C	91	VAL
6	C	95	THR
6	C	96	ARG
6	C	107	VAL
6	C	108	VAL
6	C	122	THR
6	C	139	LEU
6	C	145	ARG
6	C	146	ARG
6	C	151	THR
6	C	155	GLN
6	C	166	LYS
6	C	173	ARG
6	C	199	GLU
6	C	230	LEU
6	C	234	LEU
6	C	240	LEU
6	C	250	ASP
7	D	5	ILE
7	D	6	SER
7	D	9	ARG
7	D	10	LYS
7	D	11	LEU
7	D	16	VAL
7	D	20	GLU
7	D	21	LEU
7	D	28	GLU
7	D	50	ILE
7	D	55	VAL
7	D	65	ARG
7	D	66	ILE
7	D	68	GLU
7	D	69	LEU
7	D	71	LEU
7	D	74	GLU
7	D	80	LYS
7	D	90	ARG
7	D	91	VAL
7	D	94	ARG
7	D	101	GLN
7	D	116	ARG

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Mol	Chain	Res	Type
7	D	143	ARG
7	D	148	LYS
7	D	157	LEU
7	D	200	LYS
7	D	202	LEU
7	D	208	ILE
7	D	209	ILE
7	D	210	GLU
7	D	212	LYS
7	D	221	SER
8	E	9	LEU
8	E	19	MET
8	E	24	SER
8	E	30	ARG
8	E	51	ARG
8	E	56	LEU
8	E	57	ASN
8	E	60	GLU
8	E	65	LEU
8	E	67	GLN
8	E	68	ARG
8	E	69	HIS
8	E	77	ARG
8	E	87	MET
8	E	92	LEU
8	E	95	THR
8	E	102	VAL
8	E	108	ARG
8	E	113	ARG
8	E	115	THR
8	E	121	TYR
8	E	131	LEU
8	E	142	HIS
8	E	148	ARG
8	E	159	THR
8	E	180	LEU
8	E	189	LEU
8	E	200	ARG
8	E	208	VAL
8	E	221	ARG
8	E	224	ASN
8	E	225	VAL

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Mol	Chain	Res	Type
8	E	235	TRP
8	E	248	ILE
8	E	250	GLU
8	E	251	GLU
9	F	26	GLU
9	F	29	THR
9	F	35	ILE
9	F	42	ILE
9	F	54	GLU
9	F	57	ASP
9	F	60	LEU
9	F	70	ILE
9	F	79	TYR
9	F	86	LYS
9	F	91	ILE
9	F	93	GLU
9	F	99	LEU
9	F	108	LYS
9	F	113	VAL
9	F	126	LEU
9	F	128	ASP
9	F	129	GLN
9	F	136	VAL
9	F	141	ASN
9	F	145	ARG
9	F	164	VAL
9	F	167	LEU
9	F	169	ARG
9	F	178	THR
9	F	187	ARG
9	F	188	ASN
9	F	196	LEU
9	F	216	LYS
9	F	219	LEU
9	F	221	ARG
9	F	224	LYS
10	G	3	LEU
10	G	16	ILE
10	G	17	GLU
10	G	22	HIS
10	G	23	ARG
10	G	24	VAL

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Mol	Chain	Res	Type
10	G	25	ARG
10	G	35	GLU
10	G	51	LYS
10	G	63	MET
10	G	68	LEU
10	G	72	ARG
10	G	88	ARG
10	G	95	LYS
10	G	109	LEU
10	G	124	ILE
10	G	133	LEU
10	G	147	LEU
10	G	149	LYS
10	G	159	ARG
10	G	164	LYS
10	G	177	ARG
10	G	178	LEU
10	G	193	LEU
10	G	195	ILE
10	G	215	ARG
10	G	225	GLU
11	H	9	LEU
11	H	10	SER
11	H	19	GLN
11	H	27	LEU
11	H	30	ASN
11	H	33	GLU
11	H	48	GLU
11	H	50	GLU
11	H	51	VAL
11	H	55	LYS
11	H	58	LEU
11	H	70	TYR
11	H	72	LYS
11	H	77	LEU
11	H	80	GLU
11	H	81	LEU
11	H	87	ASP
11	H	118	LEU
11	H	123	ASP
11	H	126	LEU
11	H	129	LEU

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Mol	Chain	Res	Type
11	H	130	VAL
11	H	139	ARG
11	H	147	ASN
11	H	149	ILE
11	H	152	ILE
11	H	160	GLN
11	H	163	ASP
11	H	165	LYS
11	H	169	PHE
11	H	176	LEU
11	H	180	GLN
12	I	9	HIS
12	I	23	LYS
12	I	29	LEU
12	I	41	LYS
12	I	56	ARG
12	I	58	LEU
12	I	97	THR
12	I	104	ILE
12	I	119	GLN
12	I	121	LEU
12	I	179	ARG
12	I	196	ARG
12	I	200	LYS
13	J	3	ARG
13	J	8	TYR
13	J	17	ARG
13	J	28	LEU
13	J	33	GLU
13	J	36	LEU
13	J	37	LYS
13	J	45	ILE
13	J	49	LEU
13	J	64	GLU
13	J	65	LYS
13	J	89	ASP
13	J	100	LYS
13	J	107	ARG
13	J	109	LEU
13	J	111	THR
13	J	118	LEU
13	J	133	HIS

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Mol	Chain	Res	Type
13	J	145	SER
13	J	150	LEU
13	J	153	GLU
14	K	2	LEU
14	K	5	LYS
14	K	17	GLN
14	K	20	VAL
14	K	21	LEU
14	K	35	ILE
14	K	44	LYS
14	K	52	LYS
14	K	67	THR
14	K	76	LEU
14	K	85	HIS
14	K	86	ILE
15	L	5	LEU
15	L	6	THR
15	L	8	GLN
15	L	10	GLU
15	L	19	ILE
15	L	21	THR
15	L	36	LYS
15	L	83	THR
15	L	84	ILE
15	L	111	VAL
15	L	124	THR
15	L	136	ARG
15	L	144	SER
16	M	17	ILE
16	M	74	GLU
16	M	88	LEU
16	M	90	GLU
16	M	99	ARG
16	M	110	SER
16	M	121	THR
16	M	125	GLU
17	N	3	ARG
17	N	27	LYS
17	N	42	ARG
17	N	64	LYS
17	N	70	LYS
17	N	72	LEU

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Mol	Chain	Res	Type
17	N	88	LEU
17	N	105	ASN
17	N	106	ARG
17	N	107	LYS
17	N	109	LYS
17	N	110	ASP
17	N	112	LYS
17	N	132	VAL
17	N	142	GLU
17	N	150	VAL
18	O	13	VAL
18	O	24	ASN
18	O	49	LYS
18	O	52	ARG
18	O	90	ARG
18	O	92	LYS
18	O	110	LEU
18	O	114	ARG
18	O	124	ASP
18	O	129	LYS
19	P	13	LYS
19	P	20	VAL
19	P	28	MET
19	P	40	ARG
19	P	56	LEU
19	P	57	MET
19	P	71	GLU
19	P	72	LYS
19	P	84	ILE
19	P	119	PHE
19	P	122	THR
20	Q	13	LYS
20	Q	43	ILE
20	Q	65	ILE
20	Q	67	VAL
20	Q	83	GLN
20	Q	89	LEU
20	Q	97	VAL
20	Q	98	ASP
20	Q	104	GLU
20	Q	105	LEU
20	Q	115	THR

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Mol	Chain	Res	Type
20	Q	123	ARG
20	Q	127	LYS
20	Q	137	ARG
20	Q	139	GLN
20	Q	141	SER
21	R	3	ARG
21	R	10	LYS
21	R	29	GLN
21	R	34	LEU
21	R	46	LEU
21	R	47	ARG
21	R	48	ASN
21	R	55	THR
21	R	78	ARG
21	R	80	ARG
21	R	117	LEU
22	S	8	GLN
22	S	11	PHE
22	S	18	LEU
22	S	25	ASN
22	S	54	LEU
22	S	86	LEU
22	S	88	ARG
22	S	96	LYS
22	S	103	ASN
22	S	109	LEU
22	S	110	ARG
22	S	114	GLU
22	S	128	PHE
22	S	141	THR
22	S	144	ARG
23	T	12	GLN
23	T	16	ASN
23	T	28	LEU
23	T	29	GLU
23	T	65	ILE
23	T	79	LEU
23	T	91	HIS
23	T	103	LYS
23	T	124	ILE
23	T	129	LEU
23	T	135	ILE

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Mol	Chain	Res	Type
24	U	27	THR
24	U	83	GLU
24	U	89	ARG
24	U	91	ILE
24	U	93	LEU
25	V	1	MET
25	V	8	LEU
25	V	12	TYR
25	V	21	ASN
25	V	33	GLN
25	V	34	ILE
25	V	40	ASP
25	V	62	ARG
25	V	69	LEU
26	W	3	ARG
26	W	9	ASP
26	W	16	ASN
26	W	23	ARG
26	W	24	GLN
26	W	25	VAL
26	W	43	LYS
26	W	51	GLU
26	W	60	LYS
26	W	74	VAL
26	W	113	HIS
26	W	115	GLU
27	X	9	LEU
27	X	14	LYS
27	X	19	ARG
27	X	30	LYS
27	X	59	ILE
27	X	60	GLU
27	X	77	ILE
27	X	79	ASN
27	X	83	VAL
27	X	93	LEU
27	X	100	ASP
27	X	107	PHE
27	X	123	LYS
27	X	132	LEU
28	Y	5	ILE
28	Y	8	ARG

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Mol	Chain	Res	Type
28	Y	18	LEU
28	Y	31	ASN
28	Y	63	GLN
28	Y	69	SER
28	Y	74	LEU
28	Y	84	LYS
28	Y	99	LYS
28	Y	107	GLN
28	Y	110	GLN
28	Y	112	LYS
28	Y	127	LYS
28	Y	128	LYS
29	Z	62	VAL
29	Z	80	LEU
30	a	12	LYS
30	a	38	ARG
30	a	39	MET
30	a	64	LEU
31	b	5	GLN
31	b	8	LEU
31	b	24	LEU
31	b	31	HIS
31	b	34	ASP
31	b	57	GLU
31	b	65	THR
31	b	67	THR
32	c	16	LEU
32	c	19	THR
32	c	29	ARG
32	c	40	ILE
34	e	20	LYS
34	e	31	LYS
34	e	33	ARG
34	e	47	VAL
34	e	54	ARG
35	f	99	LYS
35	f	100	LEU
35	f	102	VAL
35	f	108	VAL
35	f	119	LYS
35	f	142	CYS
36	g	59	VAL

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Mol	Chain	Res	Type
36	g	272	LEU
37	h	8	LYS
37	h	9	ARG
38	i	23	LYS
38	i	26	LEU
38	i	31	GLU
38	i	40	LYS
38	i	56	LYS
38	i	61	ILE
38	i	62	ARG
38	i	79	VAL
38	i	85	GLN
38	i	101	ARG
39	j	7	ARG
39	j	16	ILE
39	j	19	ILE
39	j	45	MET
39	j	46	ILE
39	j	47	LEU
39	j	51	LEU
39	j	57	ARG
39	j	59	ILE
39	j	64	ARG
39	j	85	LEU
39	j	108	VAL
39	j	121	ILE
39	j	123	LEU
39	j	126	LEU
39	j	137	LYS
39	j	143	GLU
39	j	152	GLU
39	j	163	LYS
39	j	166	LEU
39	j	195	TYR
39	j	205	LEU
39	j	236	ASP
39	j	264	ILE
40	k	103	ILE
40	k	132	LEU
40	k	136	ILE
40	k	147	ILE
40	k	170	ILE

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Mol	Chain	Res	Type
40	k	188	HIS
40	k	210	VAL
40	k	223	SER
40	k	228	GLN
40	k	241	LEU
40	k	245	ILE
40	k	251	VAL
40	k	266	ILE
40	k	291	ILE
40	k	298	ILE
40	k	311	ILE
40	k	315	LEU
40	k	342	ILE
40	k	368	ILE
40	k	412	LEU
40	k	471	THR
41	l	143	ARG
41	l	165	CYS
41	l	180	ILE
41	l	186	ARG
41	l	191	LEU
41	l	198	GLU
41	l	213	ILE
41	l	227	ARG
41	l	244	THR
41	l	254	LEU
42	m	36	ARG
42	m	40	THR
42	m	54	ILE
42	m	55	LEU
42	m	96	LEU
42	m	98	LEU
42	m	104	LYS
42	m	105	ILE
43	o	18	LEU
43	o	33	ASP
43	o	42	TRP
43	o	52	VAL
43	o	56	LEU
43	o	62	LEU
43	o	73	HIS
43	o	75	TYR

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Mol	Chain	Res	Type
43	o	108	GLN
43	o	110	ARG
43	o	152	THR
43	o	183	VAL
43	o	202	LEU
43	o	206	LEU
43	o	214	ASN
43	o	229	ASP
43	o	231	ASP
43	o	232	THR
43	o	250	LEU
43	o	252	LEU
43	o	254	HIS
43	o	257	TYR
43	o	258	ARG
43	o	265	HIS
43	o	266	LEU
43	o	286	LEU
43	o	303	TRP
43	o	319	GLU
43	o	328	ILE
43	o	337	LEU
43	o	355	LEU
43	o	357	LEU
43	o	373	ASP
43	o	374	GLU
43	o	376	ILE
43	o	382	GLU
43	o	387	LEU
43	o	407	LEU
43	o	408	LEU
43	o	421	ILE
43	o	430	ARG
43	o	438	GLN
43	o	470	LEU
43	o	475	GLU
43	o	485	GLU
44	p	79	ILE
44	p	103	PHE
44	p	141	ILE
44	p	154	ARG
44	p	157	LEU

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Mol	Chain	Res	Type
44	p	233	THR
44	p	234	ASN
44	p	237	ARG
44	p	243	THR
44	p	250	GLN
44	p	278	SER
44	p	284	LEU
44	p	321	LEU
44	p	334	LEU
44	p	339	VAL
44	p	340	ARG
44	p	360	ASP
44	p	373	LEU
44	p	378	ILE
44	p	388	VAL
44	p	402	LEU
44	p	424	ARG
44	p	428	LEU
44	p	439	VAL
44	p	441	LEU
44	p	449	PHE
44	p	463	THR
44	p	468	LEU
44	p	470	ILE
44	p	471	CYS
44	p	485	LEU
44	p	500	ARG
44	p	509	VAL
44	p	528	THR
44	p	544	ILE
44	p	547	THR
44	p	551	THR
44	p	571	MET
44	p	573	ARG
44	p	579	TYR
44	p	592	ASN
44	p	599	LEU
44	p	613	ILE
44	p	623	THR
44	p	642	ILE
44	p	655	PHE
44	p	736	GLN

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Mol	Chain	Res	Type
45	q	260	THR
45	q	269	THR
45	q	278	THR
45	q	282	LEU
45	q	294	MET
45	q	298	THR
45	q	325	ILE
45	q	331	ILE
45	q	339	TYR
45	q	365	ILE
45	q	376	LEU
45	q	388	ASP
45	q	393	ASP
45	q	395	LEU
45	q	396	ILE
45	q	397	ARG
45	q	404	ILE
45	q	408	ILE
45	q	409	LEU
45	q	411	THR
45	q	413	LEU
45	q	425	LEU
45	q	431	ARG
45	q	437	LEU
45	q	438	ASP
45	q	441	TYR
45	q	448	ILE
45	q	486	LEU
45	q	488	THR
45	q	500	LYS
45	q	510	THR
45	q	524	LEU
45	q	532	ILE
45	q	535	PHE
45	q	541	ILE
45	q	542	LEU
45	q	552	LEU
45	q	557	LEU
45	q	558	CYS
45	q	561	GLU
45	q	570	LEU
45	q	590	LEU

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Mol	Chain	Res	Type
45	q	600	GLU
45	q	612	ILE
45	q	616	LEU
45	q	617	ILE
45	q	623	THR
45	q	634	THR
45	q	644	ARG
45	q	645	ILE
45	q	671	LEU
45	q	676	LEU
45	q	687	TRP
45	q	694	LEU
45	q	702	LEU
45	q	710	LEU
45	q	722	LEU
45	q	724	THR
45	q	726	PHE
45	q	744	LEU
45	q	749	GLU
45	q	764	GLU
45	q	765	ILE
45	q	774	THR
46	s	85	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (169) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	83	GLN
3	A	92	HIS
3	A	109	ASN
3	A	193	GLN
5	B	101	HIS
5	B	118	GLN
5	B	124	ASN
5	B	146	GLN
5	B	148	ASN
5	B	157	GLN
5	B	160	HIS
5	B	163	GLN
5	B	177	GLN
5	B	178	ASN
5	B	183	GLN

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Mol	Chain	Res	Type
5	B	208	GLN
5	B	211	HIS
5	B	232	HIS
6	C	94	GLN
6	C	152	ASN
6	C	155	GLN
6	C	194	GLN
6	C	214	ASN
7	D	22	ASN
7	D	101	GLN
7	D	162	GLN
8	E	67	GLN
8	E	130	GLN
8	E	224	ASN
9	F	36	GLN
9	F	39	GLN
9	F	40	GLN
9	F	129	GLN
9	F	188	ASN
10	G	10	ASN
10	G	119	GLN
10	G	185	GLN
10	G	199	GLN
11	H	19	GLN
11	H	30	ASN
11	H	71	HIS
11	H	108	GLN
11	H	110	GLN
11	H	147	ASN
11	H	164	ASN
11	H	170	GLN
11	H	180	GLN
12	I	53	GLN
12	I	94	ASN
12	I	116	HIS
13	J	142	ASN
15	L	14	GLN
15	L	22	ASN
15	L	37	ASN
15	L	118	GLN
16	M	69	GLN
16	M	76	ASN

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Mol	Chain	Res	Type
16	M	87	GLN
16	M	116	ASN
16	M	130	HIS
17	N	49	GLN
17	N	58	HIS
17	N	138	ASN
18	O	24	ASN
19	P	98	ASN
19	P	128	HIS
20	Q	8	GLN
20	Q	40	GLN
20	Q	62	ASN
20	Q	74	HIS
20	Q	83	GLN
20	Q	94	GLN
20	Q	100	GLN
21	R	29	GLN
21	R	31	ASN
21	R	62	GLN
22	S	13	HIS
22	S	44	ASN
22	S	55	HIS
22	S	89	GLN
22	S	99	HIS
22	S	136	GLN
23	T	23	GLN
23	T	43	ASN
23	T	77	ASN
24	U	44	ASN
24	U	105	GLN
25	V	3	ASN
25	V	33	GLN
25	V	38	GLN
25	V	74	GLN
26	W	92	ASN
27	X	75	GLN
27	X	79	ASN
27	X	89	ASN
28	Y	22	GLN
28	Y	77	ASN
28	Y	113	ASN
29	Z	44	GLN

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Mol	Chain	Res	Type
29	Z	98	GLN
30	a	25	ASN
31	b	26	GLN
31	b	42	ASN
32	c	27	GLN
32	c	43	ASN
33	d	5	ASN
33	d	41	GLN
34	e	17	GLN
35	f	104	ASN
35	f	132	ASN
36	g	204	ASN
36	g	210	GLN
36	g	231	ASN
36	g	234	HIS
36	g	292	GLN
38	i	33	GLN
38	i	60	HIS
38	i	106	GLN
39	j	5	HIS
39	j	23	ASN
39	j	25	GLN
39	j	103	GLN
39	j	243	GLN
40	k	98	GLN
40	k	144	ASN
40	k	188	HIS
40	k	228	GLN
40	k	249	ASN
40	k	295	ASN
40	k	376	ASN
40	k	422	HIS
41	l	193	GLN
41	l	243	ASN
42	m	67	ASN
42	m	81	GLN
42	m	99	GLN
43	o	73	HIS
43	o	172	ASN
43	o	216	GLN
43	o	222	ASN
43	o	239	GLN

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Mol	Chain	Res	Type
43	o	285	ASN
43	o	403	GLN
43	o	419	GLN
44	p	111	ASN
44	p	219	ASN
44	p	307	ASN
44	p	359	HIS
44	p	411	ASN
44	p	412	ASN
44	p	432	ASN
44	p	444	GLN
44	p	453	ASN
44	p	467	ASN
44	p	570	ASN
44	p	592	ASN
44	p	593	ASN
44	p	631	HIS
45	q	259	GLN
45	q	317	GLN
45	q	390	HIS
45	q	406	ASN
45	q	412	GLN
45	q	462	GLN
45	q	544	ASN
45	q	595	ASN
45	q	609	HIS
45	q	665	GLN
45	q	770	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	71/76 (93%)	33 (46%)	9 (12%)
2	2	1797/1798 (99%)	817 (45%)	70 (3%)
4	3	2/3 (66%)	0	0
All	All	1870/1877 (99%)	850 (45%)	79 (4%)

All (850) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	5	C

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Mol	Chain	Res	Type
1	1	9	1MG
1	1	10	2MG
1	1	11	C
1	1	12	G
1	1	16	H2U
1	1	19	G
1	1	21	A
1	1	26	M2G
1	1	27	C
1	1	29	G
1	1	31	G
1	1	32	C
1	1	34	C
1	1	35	A
1	1	37	T6A
1	1	38	A
1	1	39	C
1	1	43	G
1	1	46	7MG
1	1	47	H2U
1	1	48	5MC
1	1	49	5MC
1	1	50	U
1	1	52	G
1	1	57	G
1	1	58	1MA
1	1	61	C
1	1	64	RIA
1	1	69	C
1	1	71	C
1	1	74	C
1	1	75	C
2	2	2	A
2	2	4	C
2	2	5	U
2	2	8	U
2	2	11	A
2	2	14	C
2	2	17	C
2	2	19	A
2	2	20	G
2	2	25	C

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Mol	Chain	Res	Type
2	2	26	A
2	2	27	U
2	2	31	C
2	2	32	U
2	2	33	U
2	2	34	G
2	2	35	U
2	2	36	C
2	2	42	G
2	2	43	A
2	2	45	U
2	2	46	A
2	2	47	A
2	2	51	A
2	2	56	U
2	2	57	G
2	2	58	U
2	2	59	C
2	2	61	A
2	2	62	A
2	2	63	G
2	2	64	U
2	2	65	A
2	2	67	A
2	2	68	A
2	2	69	G
2	2	70	C
2	2	71	A
2	2	72	A
2	2	73	U
2	2	74	U
2	2	75	U
2	2	76	A
2	2	77	U
2	2	79	C
2	2	80	A
2	2	90	C
2	2	92	A
2	2	98	U
2	2	99	C
2	2	104	A
2	2	114	C

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Mol	Chain	Res	Type
2	2	116	U
2	2	119	A
2	2	120	U
2	2	123	G
2	2	124	A
2	2	127	G
2	2	128	U
2	2	129	U
2	2	130	C
2	2	131	C
2	2	132	U
2	2	133	U
2	2	134	U
2	2	135	A
2	2	136	C
2	2	137	U
2	2	138	A
2	2	139	C
2	2	140	A
2	2	144	A
2	2	146	A
2	2	147	U
2	2	152	G
2	2	156	A
2	2	157	U
2	2	158	U
2	2	159	C
2	2	160	U
2	2	167	A
2	2	169	U
2	2	176	U
2	2	183	C
2	2	187	A
2	2	188	C
2	2	189	C
2	2	190	C
2	2	191	U
2	2	193	U
2	2	194	G
2	2	196	A
2	2	202	U
2	2	208	U

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Mol	Chain	Res	Type
2	2	209	A
2	2	217	A
2	2	218	A
2	2	220	A
2	2	224	A
2	2	225	A
2	2	227	G
2	2	228	U
2	2	231	U
2	2	232	C
2	2	233	G
2	2	234	G
2	2	236	C
2	2	239	C
2	2	240	U
2	2	241	U
2	2	249	C
2	2	256	A
2	2	259	U
2	2	261	U
2	2	264	A
2	2	265	A
2	2	266	U
2	2	267	C
2	2	273	G
2	2	275	C
2	2	277	U
2	2	278	G
2	2	279	U
2	2	280	G
2	2	282	U
2	2	283	G
2	2	286	G
2	2	287	A
2	2	289	G
2	2	293	C
2	2	294	A
2	2	298	A
2	2	300	A
2	2	301	U
2	2	307	C
2	2	308	C

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Mol	Chain	Res	Type
2	2	311	A
2	2	312	U
2	2	313	C
2	2	314	A
2	2	315	A
2	2	318	U
2	2	319	U
2	2	321	G
2	2	322	A
2	2	323	U
2	2	326	U
2	2	327	A
2	2	336	G
2	2	338	C
2	2	342	C
2	2	344	U
2	2	345	G
2	2	349	U
2	2	351	A
2	2	352	A
2	2	359	A
2	2	360	C
2	2	374	U
2	2	377	A
2	2	379	U
2	2	380	C
2	2	382	G
2	2	383	G
2	2	384	A
2	2	386	A
2	2	387	G
2	2	389	G
2	2	390	A
2	2	398	A
2	2	399	A
2	2	400	A
2	2	401	C
2	2	402	G
2	2	403	G
2	2	404	C
2	2	410	C
2	2	412	U

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Mol	Chain	Res	Type
2	2	413	C
2	2	415	A
2	2	416	A
2	2	417	G
2	2	421	G
2	2	422	G
2	2	423	C
2	2	424	A
2	2	425	G
2	2	437	A
2	2	438	U
2	2	439	U
2	2	440	A
2	2	442	C
2	2	443	C
2	2	447	C
2	2	448	C
2	2	450	A
2	2	451	A
2	2	452	U
2	2	455	A
2	2	456	G
2	2	467	A
2	2	468	C
2	2	469	A
2	2	473	A
2	2	476	A
2	2	480	A
2	2	482	A
2	2	484	A
2	2	485	G
2	2	489	C
2	2	490	C
2	2	491	A
2	2	492	U
2	2	493	U
2	2	495	G
2	2	496	G
2	2	498	U
2	2	499	C
2	2	501	U
2	2	502	G

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Mol	Chain	Res	Type
2	2	503	U
2	2	504	A
2	2	505	A
2	2	506	U
2	2	507	U
2	2	510	A
2	2	512	U
2	2	516	U
2	2	517	A
2	2	518	C
2	2	519	A
2	2	522	G
2	2	524	A
2	2	525	A
2	2	527	U
2	2	531	U
2	2	533	A
2	2	534	A
2	2	535	C
2	2	536	G
2	2	537	A
2	2	538	G
2	2	539	G
2	2	540	A
2	2	541	A
2	2	542	C
2	2	543	A
2	2	545	C
2	2	547	G
2	2	548	G
2	2	553	C
2	2	554	A
2	2	556	G
2	2	557	U
2	2	558	C
2	2	560	G
2	2	562	U
2	2	564	C
2	2	565	C
2	2	566	A
2	2	568	C
2	2	569	A

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Mol	Chain	Res	Type
2	2	571	C
2	2	573	G
2	2	577	U
2	2	578	A
2	2	580	U
2	2	581	U
2	2	582	C
2	2	584	A
2	2	585	G
2	2	592	U
2	2	593	A
2	2	594	G
2	2	605	A
2	2	610	U
2	2	612	G
2	2	614	A
2	2	618	A
2	2	619	A
2	2	620	A
2	2	622	A
2	2	634	A
2	2	636	C
2	2	637	U
2	2	638	U
2	2	639	U
2	2	641	G
2	2	642	G
2	2	647	G
2	2	650	G
2	2	652	C
2	2	653	C
2	2	656	U
2	2	657	C
2	2	659	G
2	2	661	C
2	2	663	U
2	2	664	U
2	2	665	A
2	2	669	C
2	2	671	C
2	2	672	G
2	2	673	C

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Mol	Chain	Res	Type
2	2	675	C
2	2	679	U
2	2	680	U
2	2	681	U
2	2	684	A
2	2	685	A
2	2	686	C
2	2	688	G
2	2	691	U
2	2	693	U
2	2	694	U
2	2	695	U
2	2	696	C
2	2	697	C
2	2	698	U
2	2	699	U
2	2	700	C
2	2	701	U
2	2	704	C
2	2	707	A
2	2	709	C
2	2	710	U
2	2	711	G
2	2	712	U
2	2	713	A
2	2	714	C
2	2	715	U
2	2	716	C
2	2	717	C
2	2	718	U
2	2	719	U
2	2	721	U
2	2	722	G
2	2	723	G
2	2	724	G
2	2	725	U
2	2	727	C
2	2	728	A
2	2	730	G
2	2	731	C
2	2	732	G
2	2	733	A

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Mol	Chain	Res	Type
2	2	734	A
2	2	736	C
2	2	738	G
2	2	739	G
2	2	742	U
2	2	743	U
2	2	748	U
2	2	753	A
2	2	755	A
2	2	762	A
2	2	765	G
2	2	766	U
2	2	767	U
2	2	768	C
2	2	771	A
2	2	773	C
2	2	774	A
2	2	776	G
2	2	778	G
2	2	780	A
2	2	781	A
2	2	782	G
2	2	783	C
2	2	784	U
2	2	785	C
2	2	786	G
2	2	788	A
2	2	791	U
2	2	792	A
2	2	793	U
2	2	794	U
2	2	798	A
2	2	799	U
2	2	806	A
2	2	808	G
2	2	809	G
2	2	810	A
2	2	811	A
2	2	813	A
2	2	814	G
2	2	817	C
2	2	818	G

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Mol	Chain	Res	Type
2	2	819	U
2	2	820	U
2	2	821	U
2	2	822	G
2	2	823	G
2	2	825	U
2	2	826	C
2	2	827	U
2	2	828	A
2	2	829	U
2	2	830	U
2	2	832	U
2	2	840	U
2	2	843	A
2	2	845	G
2	2	851	C
2	2	855	A
2	2	856	U
2	2	857	G
2	2	859	U
2	2	861	A
2	2	862	A
2	2	863	U
2	2	872	U
2	2	875	G
2	2	881	U
2	2	891	A
2	2	897	A
2	2	898	G
2	2	901	G
2	2	902	U
2	2	903	G
2	2	905	A
2	2	907	U
2	2	908	U
2	2	910	U
2	2	911	U
2	2	912	G
2	2	913	G
2	2	914	A
2	2	915	U
2	2	919	U

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Mol	Chain	Res	Type
2	2	920	U
2	2	924	G
2	2	925	A
2	2	930	C
2	2	931	U
2	2	932	A
2	2	933	C
2	2	934	U
2	2	939	A
2	2	941	G
2	2	942	C
2	2	944	U
2	2	946	U
2	2	947	G
2	2	950	A
2	2	956	G
2	2	958	U
2	2	965	A
2	2	968	C
2	2	972	A
2	2	976	A
2	2	977	A
2	2	982	A
2	2	983	G
2	2	984	G
2	2	987	A
2	2	991	A
2	2	994	A
2	2	995	U
2	2	999	C
2	2	1000	A
2	2	1001	G
2	2	1002	A
2	2	1003	U
2	2	1004	A
2	2	1006	C
2	2	1011	U
2	2	1015	C
2	2	1016	U
2	2	1018	A
2	2	1019	A
2	2	1022	A

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Mol	Chain	Res	Type
2	2	1023	U
2	2	1024	A
2	2	1025	A
2	2	1026	A
2	2	1027	C
2	2	1028	U
2	2	1029	A
2	2	1030	U
2	2	1031	G
2	2	1034	G
2	2	1038	A
2	2	1041	G
2	2	1047	G
2	2	1048	U
2	2	1049	G
2	2	1050	G
2	2	1051	U
2	2	1052	G
2	2	1054	U
2	2	1055	U
2	2	1056	U
2	2	1057	U
2	2	1058	C
2	2	1059	U
2	2	1062	U
2	2	1070	U
2	2	1073	G
2	2	1081	C
2	2	1082	G
2	2	1084	G
2	2	1090	A
2	2	1091	A
2	2	1093	G
2	2	1095	C
2	2	1096	U
2	2	1097	U
2	2	1099	G
2	2	1100	G
2	2	1102	U
2	2	1103	U
2	2	1105	U
2	2	1112	A

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Mol	Chain	Res	Type
2	2	1113	G
2	2	1114	U
2	2	1118	G
2	2	1123	A
2	2	1124	A
2	2	1130	A
2	2	1136	A
2	2	1137	A
2	2	1142	A
2	2	1145	G
2	2	1146	A
2	2	1149	G
2	2	1156	A
2	2	1157	C
2	2	1158	C
2	2	1161	C
2	2	1162	A
2	2	1166	G
2	2	1168	G
2	2	1176	C
2	2	1179	C
2	2	1182	A
2	2	1183	A
2	2	1184	U
2	2	1186	U
2	2	1188	A
2	2	1190	U
2	2	1191	C
2	2	1192	A
2	2	1193	A
2	2	1195	A
2	2	1198	G
2	2	1199	G
2	2	1200	G
2	2	1201	A
2	2	1202	A
2	2	1203	A
2	2	1204	C
2	2	1205	U
2	2	1207	A
2	2	1208	C
2	2	1212	G

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Mol	Chain	Res	Type
2	2	1213	U
2	2	1215	C
2	2	1216	A
2	2	1217	G
2	2	1218	A
2	2	1224	U
2	2	1227	G
2	2	1228	G
2	2	1229	A
2	2	1232	G
2	2	1238	U
2	2	1240	G
2	2	1241	A
2	2	1242	G
2	2	1243	A
2	2	1244	G
2	2	1245	C
2	2	1250	U
2	2	1255	A
2	2	1258	U
2	2	1260	G
2	2	1264	G
2	2	1265	U
2	2	1266	G
2	2	1268	U
2	2	1269	G
2	2	1270	G
2	2	1271	U
2	2	1272	G
2	2	1277	G
2	2	1278	C
2	2	1279	C
2	2	1281	U
2	2	1282	U
2	2	1283	C
2	2	1284	U
2	2	1285	U
2	2	1292	U
2	2	1295	A
2	2	1296	G
2	2	1298	G
2	2	1299	A

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Mol	Chain	Res	Type
2	2	1305	C
2	2	1306	U
2	2	1310	U
2	2	1313	U
2	2	1314	U
2	2	1315	G
2	2	1316	C
2	2	1318	A
2	2	1319	U
2	2	1320	A
2	2	1321	A
2	2	1322	C
2	2	1323	G
2	2	1324	A
2	2	1332	C
2	2	1336	A
2	2	1338	C
2	2	1339	U
2	2	1343	A
2	2	1344	A
2	2	1345	A
2	2	1347	A
2	2	1350	G
2	2	1351	U
2	2	1356	G
2	2	1357	G
2	2	1360	C
2	2	1362	U
2	2	1363	G
2	2	1364	C
2	2	1369	U
2	2	1370	G
2	2	1371	A
2	2	1372	C
2	2	1374	C
2	2	1375	U
2	2	1376	U
2	2	1378	U
2	2	1380	A
2	2	1381	G
2	2	1382	A
2	2	1384	G

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Mol	Chain	Res	Type
2	2	1386	A
2	2	1388	U
2	2	1393	G
2	2	1395	U
2	2	1396	U
2	2	1397	C
2	2	1398	A
2	2	1400	G
2	2	1401	C
2	2	1404	A
2	2	1406	G
2	2	1410	G
2	2	1411	U
2	2	1412	U
2	2	1413	U
2	2	1414	G
2	2	1415	A
2	2	1416	G
2	2	1419	A
2	2	1420	A
2	2	1425	A
2	2	1426	G
2	2	1429	C
2	2	1430	U
2	2	1431	G
2	2	1432	U
2	2	1433	G
2	2	1434	A
2	2	1442	A
2	2	1443	G
2	2	1444	A
2	2	1445	C
2	2	1446	G
2	2	1448	U
2	2	1452	G
2	2	1453	G
2	2	1455	C
2	2	1456	G
2	2	1457	C
2	2	1460	G
2	2	1463	C
2	2	1464	G

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Mol	Chain	Res	Type
2	2	1467	A
2	2	1469	A
2	2	1471	U
2	2	1476	G
2	2	1479	C
2	2	1482	G
2	2	1483	C
2	2	1484	G
2	2	1488	A
2	2	1489	C
2	2	1490	A
2	2	1491	A
2	2	1492	C
2	2	1494	U
2	2	1495	U
2	2	1496	G
2	2	1498	C
2	2	1499	C
2	2	1501	A
2	2	1502	G
2	2	1504	G
2	2	1507	C
2	2	1509	G
2	2	1512	U
2	2	1513	A
2	2	1514	A
2	2	1515	U
2	2	1516	C
2	2	1519	G
2	2	1520	U
2	2	1521	G
2	2	1522	A
2	2	1523	A
2	2	1526	U
2	2	1528	C
2	2	1529	G
2	2	1532	G
2	2	1533	U
2	2	1534	G
2	2	1535	C
2	2	1536	U
2	2	1538	G

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Mol	Chain	Res	Type
2	2	1549	U
2	2	1554	A
2	2	1555	U
2	2	1557	A
2	2	1570	G
2	2	1571	A
2	2	1572	G
2	2	1573	G
2	2	1575	A
2	2	1576	U
2	2	1579	C
2	2	1580	U
2	2	1581	A
2	2	1583	U
2	2	1584	A
2	2	1588	G
2	2	1594	C
2	2	1595	A
2	2	1597	C
2	2	1598	A
2	2	1599	G
2	2	1604	C
2	2	1613	C
2	2	1614	G
2	2	1623	C
2	2	1625	U
2	2	1628	U
2	2	1630	C
2	2	1632	C
2	2	1633	A
2	2	1635	C
2	2	1638	C
2	2	1640	G
2	2	1649	A
2	2	1655	U
2	2	1656	G
2	2	1662	C
2	2	1673	C
2	2	1676	A
2	2	1678	G
2	2	1679	A
2	2	1682	U

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Mol	Chain	Res	Type
2	2	1686	U
2	2	1687	A
2	2	1688	G
2	2	1692	A
2	2	1693	G
2	2	1694	G
2	2	1695	G
2	2	1696	G
2	2	1697	G
2	2	1698	C
2	2	1700	A
2	2	1701	C
2	2	1702	U
2	2	1703	C
2	2	1704	C
2	2	1705	A
2	2	1706	U
2	2	1707	C
2	2	1708	U
2	2	1709	C
2	2	1710	A
2	2	1711	G
2	2	1712	A
2	2	1715	G
2	2	1719	A
2	2	1724	G
2	2	1725	G
2	2	1728	A
2	2	1742	A
2	2	1748	A
2	2	1752	A
2	2	1753	A
2	2	1754	A
2	2	1758	G
2	2	1763	A
2	2	1764	A
2	2	1767	U
2	2	1768	U
2	2	1777	U
2	2	1778	G
2	2	1781	C
2	2	1787	G

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Mol	Chain	Res	Type
2	2	1789	A
2	2	1790	G
2	2	1791	G
2	2	1792	A
2	2	1793	U
2	2	1794	C
2	2	1796	U
2	2	1797	U
2	2	1798	A

All (79) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	9	1MG
1	1	10	2MG
1	1	20	A
1	1	26	M2G
1	1	46	7MG
1	1	47	H2U
1	1	48	5MC
1	1	49	5MC
1	1	74	C
2	2	25	C
2	2	58	U
2	2	61	A
2	2	68	A
2	2	74	U
2	2	115	G
2	2	130	C
2	2	140	A
2	2	191	U
2	2	216	A
2	2	217	A
2	2	239	C
2	2	258	U
2	2	265	A
2	2	277	U
2	2	279	U
2	2	318	U
2	2	321	G
2	2	344	U
2	2	437	A

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Mol	Chain	Res	Type
2	2	524	A
2	2	538	G
2	2	542	C
2	2	557	U
2	2	564	C
2	2	637	U
2	2	649	U
2	2	670	G
2	2	685	A
2	2	695	U
2	2	700	C
2	2	721	U
2	2	735	C
2	2	742	U
2	2	765	G
2	2	812	U
2	2	822	G
2	2	828	A
2	2	854	A
2	2	896	C
2	2	907	U
2	2	912	G
2	2	938	A
2	2	946	U
2	2	1001	G
2	2	1030	U
2	2	1051	U
2	2	1107	G
2	2	1123	A
2	2	1149	G
2	2	1198	G
2	2	1206	C
2	2	1314	U
2	2	1343	A
2	2	1386	A
2	2	1410	G
2	2	1411	U
2	2	1430	U
2	2	1445	C
2	2	1455	C
2	2	1487	U
2	2	1491	A

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Mol	Chain	Res	Type
2	2	1534	G
2	2	1571	A
2	2	1580	U
2	2	1613	C
2	2	1678	G
2	2	1789	A
2	2	1792	A
2	2	1795	A

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

11 non-standard protein/DNA/RNA residues are modelled in this entry.

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
1	H2U	1	47	1	18,21,22	0.73	0	19,30,33	1.36	2 (10%)
1	1MA	1	58	1	21,25,26	1.54	4 (19%)	30,37,40	1.87	5 (16%)
1	H2U	1	16	1	18,21,22	0.82	0	19,30,33	1.47	4 (21%)
1	1MG	1	9	1	23,26,27	1.45	3 (13%)	33,39,42	2.09	9 (27%)
1	T6A	1	37	1	31,34,35	1.54	4 (12%)	43,49,52	2.30	13 (30%)
1	RIA	1	64	1	35,38,39	1.34	4 (11%)	50,57,60	1.96	11 (22%)
1	2MG	1	10	1	23,26,27	1.35	4 (17%)	33,38,41	2.31	7 (21%)
1	7MG	1	46	1	23,26,27	1.49	4 (17%)	27,39,42	2.66	7 (25%)
1	M2G	1	26	1	24,27,28	1.40	4 (16%)	33,40,43	2.03	7 (21%)
1	5MC	1	49	1	19,22,23	2.33	4 (21%)	26,32,35	1.53	2 (7%)
1	5MC	1	48	1	19,22,23	1.94	1 (5%)	26,32,35	1.54	6 (23%)

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
1	H2U	1	47	1	-	5/7/38/39	0/2/2/2
1	1MA	1	58	1	-	2/7/25/26	0/3/3/3
1	H2U	1	16	1	-	2/7/38/39	0/2/2/2
1	1MG	1	9	1	-	3/7/25/26	0/3/3/3
1	T6A	1	37	1	-	11/23/41/42	0/3/3/3
1	RIA	1	64	1	-	9/17/51/52	0/4/4/4
1	2MG	1	10	1	-	2/9/27/28	0/3/3/3
1	7MG	1	46	1	-	2/7/37/38	0/3/3/3
1	M2G	1	26	1	-	5/11/29/30	0/3/3/3
1	5MC	1	49	1	-	1/7/25/26	0/2/2/2
1	5MC	1	48	1	-	0/7/25/26	0/2/2/2

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	49	5MC	C5-C4	8.24	1.50	1.44
1	1	48	5MC	C5-C4	7.24	1.49	1.44
1	1	37	T6A	C5-C4	5.48	1.48	1.39
1	1	64	RIA	C5-C4	5.16	1.48	1.39
1	1	26	M2G	C2-N2	3.73	1.42	1.35
1	1	46	7MG	C5-C4	3.72	1.49	1.37
1	1	58	1MA	C6-N6	3.59	1.36	1.28
1	1	9	1MG	C2-N1	3.58	1.43	1.37
1	1	10	2MG	C5-C4	3.54	1.48	1.38
1	1	58	1MA	C5-C4	3.54	1.48	1.38
1	1	9	1MG	C5-C4	3.54	1.48	1.38
1	1	37	T6A	C5-C6	3.48	1.50	1.41
1	1	26	M2G	C5-C4	3.31	1.47	1.38
1	1	49	5MC	C6-C5	3.13	1.39	1.34
1	1	10	2MG	C2-N3	2.81	1.37	1.32
1	1	64	RIA	C5-C6	2.81	1.48	1.41
1	1	58	1MA	C2-N3	2.78	1.35	1.30
1	1	46	7MG	C8-N9	2.67	1.47	1.45
1	1	64	RIA	C5-N7	-2.45	1.34	1.39
1	1	64	RIA	C8-N7	2.44	1.36	1.31
1	1	37	T6A	C8-N7	2.42	1.36	1.31
1	1	46	7MG	C1'-N9	2.41	1.51	1.46
1	1	46	7MG	C5-C6	2.31	1.49	1.43
1	1	58	1MA	C5-C6	2.30	1.49	1.43
1	1	37	T6A	C5-N7	-2.17	1.35	1.39
1	1	9	1MG	C5-N7	-2.17	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	26	M2G	C5-N7	-2.14	1.34	1.39
1	1	26	M2G	C2-N3	2.08	1.37	1.32
1	1	49	5MC	O2-C2	2.07	1.27	1.23
1	1	49	5MC	O4'-C1'	-2.06	1.37	1.42
1	1	10	2MG	C5-N7	-2.02	1.35	1.39
1	1	10	2MG	C6-N1	-2.02	1.35	1.38

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	46	7MG	N9-C4-N3	8.78	138.32	125.46
1	1	10	2MG	C2-N3-C4	7.93	121.91	112.00
1	1	10	2MG	C5-C4-N3	-6.41	118.18	128.39
1	1	26	M2G	C5-C4-N3	-6.28	118.39	128.39
1	1	37	T6A	C5-C4-N3	-6.15	118.25	126.72
1	1	37	T6A	N6-C10-N11	5.96	121.97	113.77
1	1	9	1MG	C5-C4-N3	-5.95	118.91	128.39
1	1	46	7MG	C5-C4-N3	-5.85	117.15	128.13
1	1	64	RIA	C5-C4-N3	-5.64	118.96	126.72
1	1	58	1MA	C5-C4-N3	-5.60	119.02	127.27
1	1	26	M2G	C2-N3-C4	5.27	122.26	112.51
1	1	46	7MG	C2-N3-C4	5.00	120.91	112.30
1	1	58	1MA	C2-N3-C4	4.93	122.20	112.53
1	1	9	1MG	C2-N3-C4	4.87	122.93	111.98
1	1	64	RIA	N3-C4-N9	4.75	135.25	127.17
1	1	64	RIA	C2A-C1A-N9	-4.65	106.10	113.75
1	1	37	T6A	N3-C4-N9	4.52	134.86	127.17
1	1	10	2MG	N9-C4-N3	4.48	134.91	125.95
1	1	26	M2G	N9-C4-N3	4.45	134.84	125.95
1	1	49	5MC	O2-C2-N3	-4.39	115.42	122.33
1	1	9	1MG	N9-C4-N3	4.34	134.63	125.95
1	1	46	7MG	N9-C8-N7	-4.14	97.52	103.37
1	1	37	T6A	C4-C5-N7	-4.06	105.94	110.58
1	1	37	T6A	O10-C10-N6	-4.03	116.48	123.64
1	1	37	T6A	C2-N3-C4	3.84	121.21	111.83
1	1	64	RIA	C2-N3-C4	3.81	121.15	111.83
1	1	37	T6A	N3-C2-N1	-3.61	123.12	128.58
1	1	48	5MC	C3'-C2'-C1'	3.55	108.18	101.46
1	1	16	H2U	O4'-C1'-N1	3.48	114.05	109.30
1	1	64	RIA	N3-C2-N1	-3.47	123.33	128.58
1	1	58	1MA	N9-C4-N3	3.47	134.81	126.90
1	1	10	2MG	C6-C5-N7	3.45	136.56	130.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	37	T6A	C6-C5-N7	3.43	136.16	132.43
1	1	48	5MC	C5-C4-N3	-3.42	118.25	121.75
1	1	26	M2G	C6-C5-N7	3.29	136.28	130.29
1	1	64	RIA	C1'-C2'-C3'	3.21	106.29	102.29
1	1	37	T6A	C5-C6-N6	3.21	127.12	118.94
1	1	9	1MG	C3'-C2'-C1'	3.08	107.30	101.46
1	1	47	H2U	O4'-C1'-N1	3.07	113.48	109.30
1	1	64	RIA	C4-C5-N7	-3.06	107.09	110.58
1	1	46	7MG	C5-C6-N1	2.95	116.12	110.94
1	1	9	1MG	N2-C2-N1	2.89	121.11	118.79
1	1	10	2MG	C4-C5-N7	-2.80	106.24	110.67
1	1	9	1MG	C4-C5-N7	-2.76	106.30	110.67
1	1	37	T6A	C5-N7-C8	2.75	107.77	103.45
1	1	47	H2U	C5-C4-N3	2.72	119.58	116.69
1	1	64	RIA	C5-N7-C8	2.69	107.67	103.45
1	1	26	M2G	C4-C5-N7	-2.66	106.46	110.67
1	1	16	H2U	C5-C4-N3	2.63	119.48	116.69
1	1	37	T6A	O4'-C1'-N9	2.62	113.12	108.09
1	1	48	5MC	O2-C2-N3	-2.62	118.20	122.33
1	1	9	1MG	C6-C5-N7	2.61	135.16	129.36
1	1	58	1MA	C4-C5-N7	-2.45	106.79	110.67
1	1	37	T6A	C12-N11-C10	2.44	126.04	121.99
1	1	37	T6A	C2-N1-C6	2.40	123.19	115.24
1	1	48	5MC	C4'-O4'-C1'	2.37	114.69	109.47
1	1	16	H2U	C3'-C2'-C1'	2.35	105.92	101.46
1	1	26	M2G	C3'-C2'-C1'	2.33	105.88	101.46
1	1	46	7MG	C3'-C2'-C1'	2.31	105.83	101.46
1	1	10	2MG	C3'-C2'-C1'	2.26	105.75	101.46
1	1	64	RIA	C2A-C3A-C4A	2.23	106.78	101.99
1	1	49	5MC	N1-C2-N3	2.21	122.64	118.80
1	1	48	5MC	CM5-C5-C6	-2.20	119.87	122.85
1	1	16	H2U	C5-C6-N1	-2.19	104.88	111.52
1	1	58	1MA	C6-C5-N7	2.19	136.03	132.16
1	1	64	RIA	C4-N9-C8	2.12	107.96	105.74
1	1	26	M2G	O6-C6-C5	-2.11	120.95	126.53
1	1	48	5MC	C2'-C3'-C4'	2.09	106.65	102.61
1	1	46	7MG	O4'-C1'-N9	2.08	112.13	109.30
1	1	64	RIA	O1'-C1'-C2'	2.08	107.62	104.98
1	1	9	1MG	C2-N1-C6	-2.01	119.31	120.99
1	1	9	1MG	O6-C6-C5	-2.01	119.42	124.59
1	1	10	2MG	O6-C6-C5	-2.00	121.24	126.53

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	16	H2U	O4'-C4'-C5'-O5'
1	1	26	M2G	N1-C2-N2-CM1
1	1	26	M2G	N3-C2-N2-CM1
1	1	26	M2G	N3-C2-N2-CM2
1	1	37	T6A	O4'-C4'-C5'-O5'
1	1	37	T6A	O4'-C1'-N9-C8
1	1	37	T6A	O4'-C1'-N9-C4
1	1	37	T6A	C13-C12-C14-O14
1	1	37	T6A	C13-C12-C14-C15
1	1	46	7MG	C3'-C4'-C5'-O5'
1	1	47	H2U	O4'-C1'-N1-C2
1	1	47	H2U	O4'-C1'-N1-C6
1	1	58	1MA	O4'-C4'-C5'-O5'
1	1	58	1MA	C3'-C4'-C5'-O5'
1	1	64	RIA	O1'-C1'-O2A-C2A
1	1	64	RIA	C2'-C1'-O2A-C2A
1	1	64	RIA	C4'-C5'-O5'-P'
1	1	9	1MG	O4'-C4'-C5'-O5'
1	1	10	2MG	O4'-C4'-C5'-O5'
1	1	37	T6A	C3'-C4'-C5'-O5'
1	1	47	H2U	O4'-C4'-C5'-O5'
1	1	10	2MG	C3'-C4'-C5'-O5'
1	1	46	7MG	O4'-C4'-C5'-O5'
1	1	47	H2U	C3'-C4'-C5'-O5'
1	1	9	1MG	C3'-C4'-C5'-O5'
1	1	16	H2U	C3'-C4'-C5'-O5'
1	1	47	H2U	C4'-C5'-O5'-P
1	1	37	T6A	N11-C12-C14-O14
1	1	64	RIA	C3'-C4'-C5'-O5'
1	1	26	M2G	C3'-C4'-C5'-O5'
1	1	37	T6A	C4'-C5'-O5'-P
1	1	26	M2G	N1-C2-N2-CM2
1	1	37	T6A	N11-C12-C14-C15
1	1	37	T6A	N1-C6-N6-C10
1	1	64	RIA	C2A-C1A-N9-C8
1	1	9	1MG	C4'-C5'-O5'-P
1	1	49	5MC	C4'-C5'-O5'-P
1	1	64	RIA	C2A-C1A-N9-C4
1	1	37	T6A	C5-C6-N6-C10
1	1	64	RIA	C4A-C5A-O5A-P
1	1	64	RIA	O1'-C4'-C5'-O5'
1	1	64	RIA	C3A-C2A-O2A-C1'

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	16	H2U	1	0
1	1	64	RIA	2	0
1	1	48	5MC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 88 ligands modelled in this entry, 86 are monoatomic - leaving 2 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
51	GCP	k	602	49	32,34,34	1.56	7 (21%)	49,54,54	1.82	7 (14%)
48	7NO	1	101	1	29,32,33	1.42	1 (3%)	38,45,48	5.21	3 (7%)

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
51	GCP	k	602	49	-	7/19/38/38	0/3/3/3
48	7NO	1	101	1	-	6/19/37/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	1	101	7NO	O3'-C	7.35	1.51	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	k	602	GCP	C5-C4	3.46	1.48	1.38
51	k	602	GCP	PG-O2G	3.27	1.62	1.55
51	k	602	GCP	PA-O3A	3.18	1.62	1.59
51	k	602	GCP	PB-O3A	2.84	1.61	1.58
51	k	602	GCP	PG-O3G	2.57	1.60	1.55
51	k	602	GCP	C6-N1	-2.10	1.34	1.38
51	k	602	GCP	PB-O2B	2.09	1.61	1.56

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	1	101	7NO	C3'-O3'-C	25.27	159.74	117.76
48	1	101	7NO	O3'-C-O	-16.42	94.30	123.95
48	1	101	7NO	O3'-C-CA	10.78	135.89	111.41
51	k	602	GCP	C5-C4-N3	-6.67	117.78	128.39
51	k	602	GCP	C2-N3-C4	5.48	121.74	112.30
51	k	602	GCP	N9-C4-N3	5.02	135.99	125.95
51	k	602	GCP	C6-C5-N7	3.15	136.02	130.29
51	k	602	GCP	C4-C5-N7	-2.60	106.55	110.67
51	k	602	GCP	C3'-C2'-C1'	2.22	105.66	101.46
51	k	602	GCP	O6-C6-C5	-2.06	121.10	126.53

There are no chirality outliers.

All (13) torsion outliers are listed below:

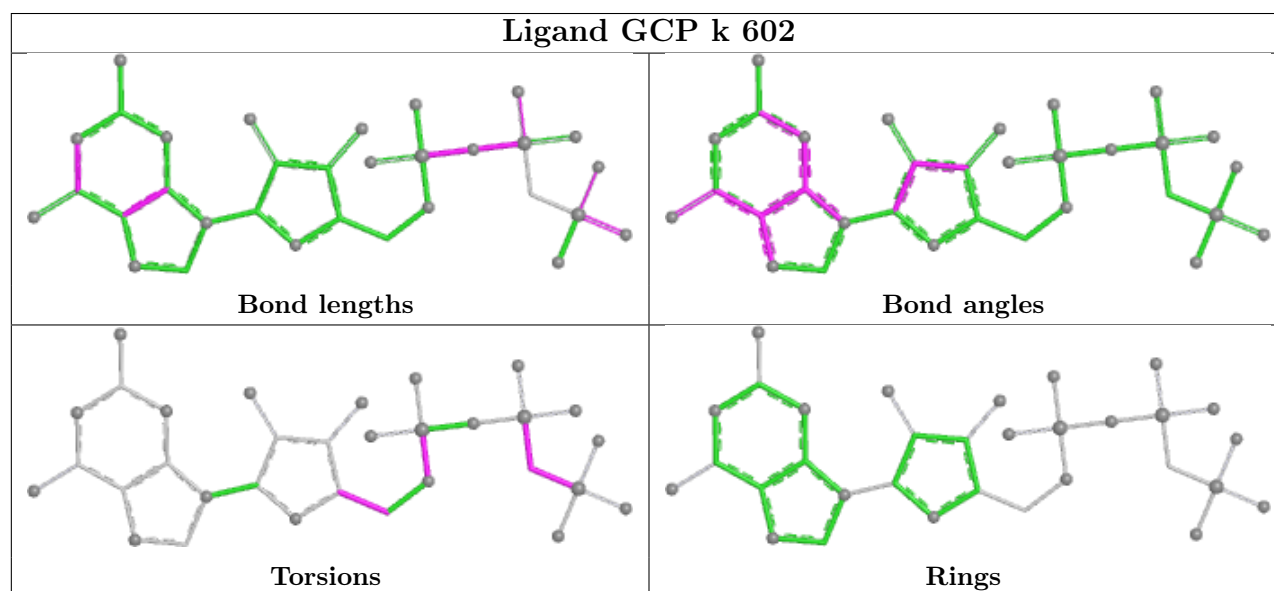
Mol	Chain	Res	Type	Atoms
48	1	101	7NO	C4'-C3'-O3'-C
48	1	101	7NO	CA-C-O3'-C3'
48	1	101	7NO	O-C-O3'-C3'
51	k	602	GCP	PG-C3B-PB-O2B
51	k	602	GCP	C5'-O5'-PA-O1A
51	k	602	GCP	O4'-C4'-C5'-O5'
51	k	602	GCP	C3'-C4'-C5'-O5'
48	1	101	7NO	O4'-C4'-C5'-O5'
48	1	101	7NO	C3'-C4'-C5'-O5'
48	1	101	7NO	O3'-C-CA-N
51	k	602	GCP	C5'-O5'-PA-O3A
51	k	602	GCP	PG-C3B-PB-O1B
51	k	602	GCP	PB-C3B-PG-O1G

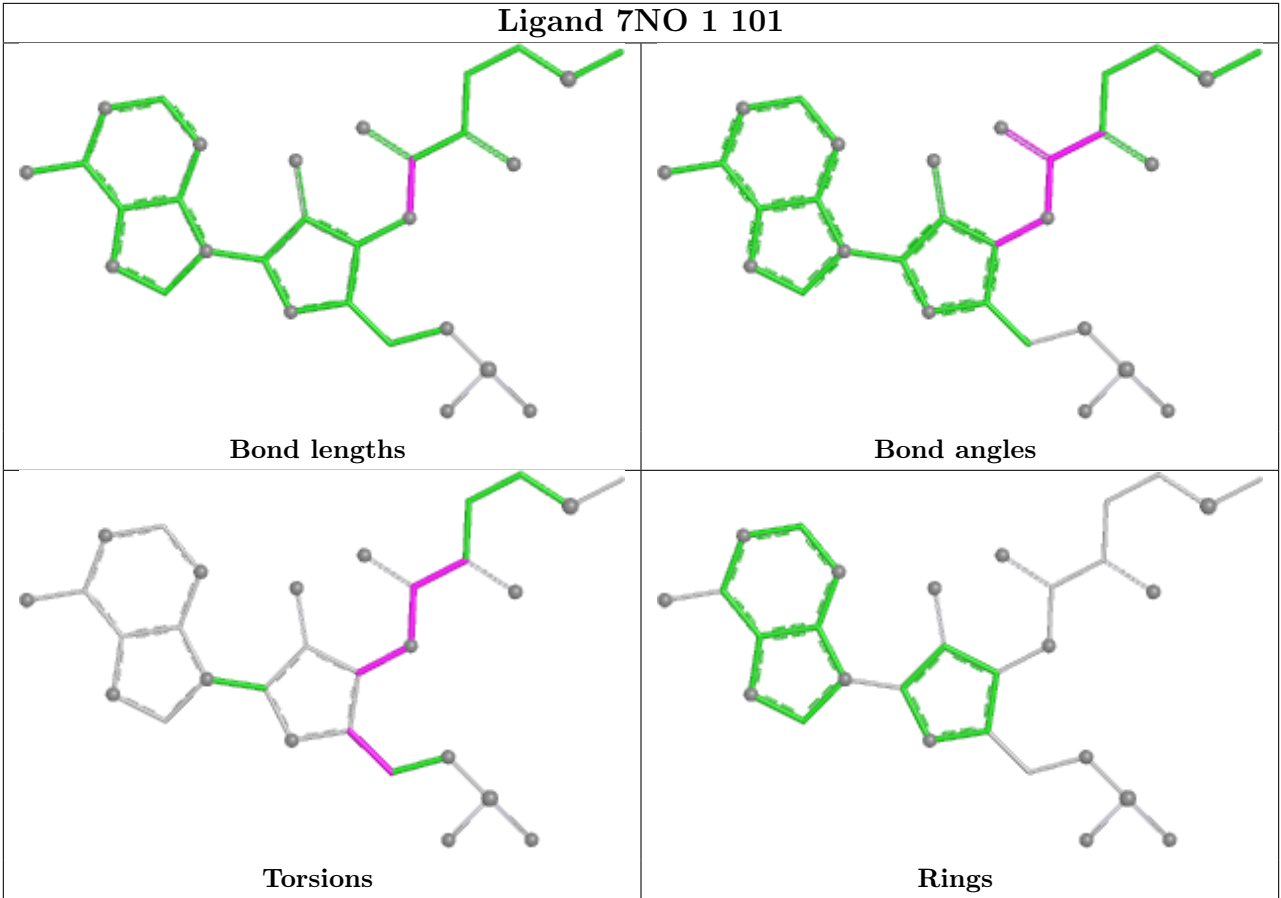
There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
51	k	602	GCP	6	0
48	1	101	7NO	3	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
45	q	3
44	p	3
1	1	2
43	o	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	o	492:ALA	C	693:UNK	N	236.15
1	q	219:ASP	C	251:GLN	N	49.57
1	q	186:LEU	C	189:LYS	N	9.27

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	p	700:ARG	C	705:HIS	N	8.32
1	l	64:RIA	O3'	65:G	P	6.22
1	p	684:SER	C	688:GLU	N	5.94
1	l	16:H2U	O3'	18:G	P	5.10
1	p	664:PRO	C	668:LEU	N	5.10
1	q	137:ASP	C	139:TRP	N	3.87

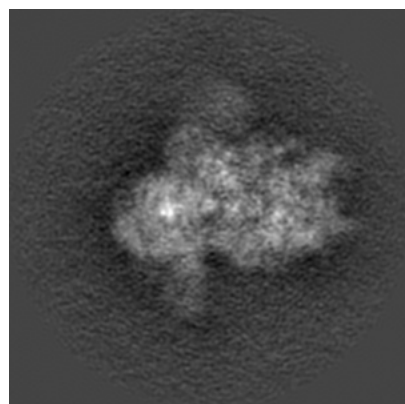
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0057. These allow visual inspection of the internal detail of the map and identification of artifacts.

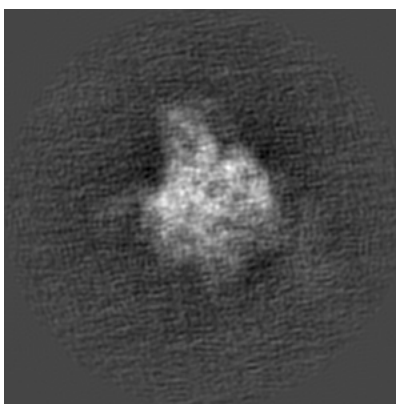
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

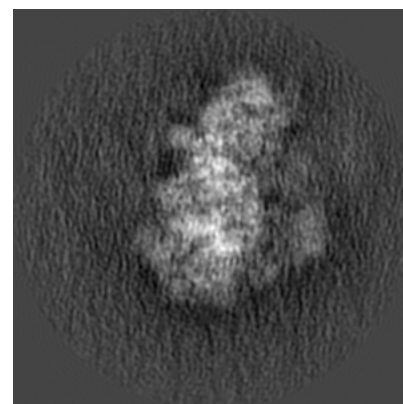
6.1.1 Primary map



X

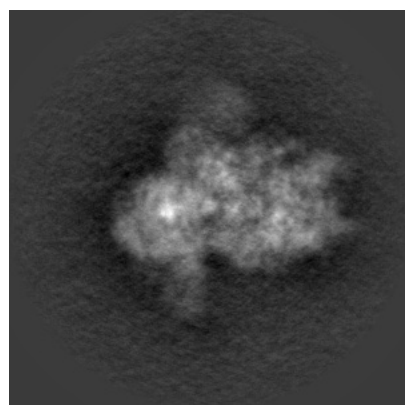


Y

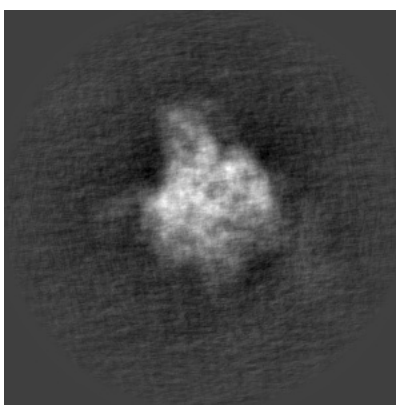


Z

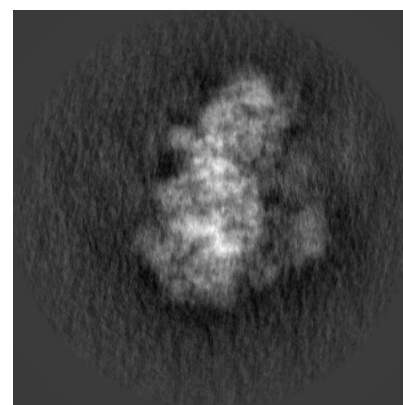
6.1.2 Raw map



X



Y

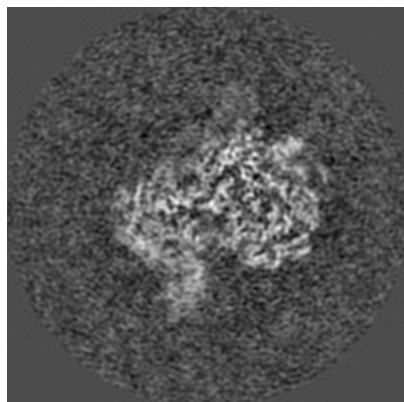


Z

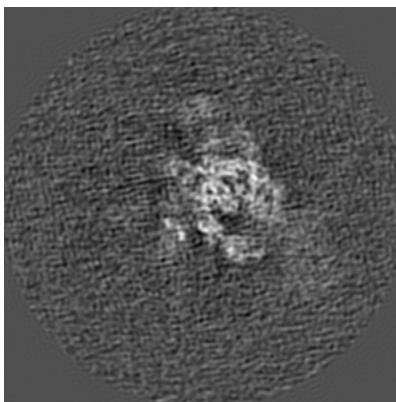
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

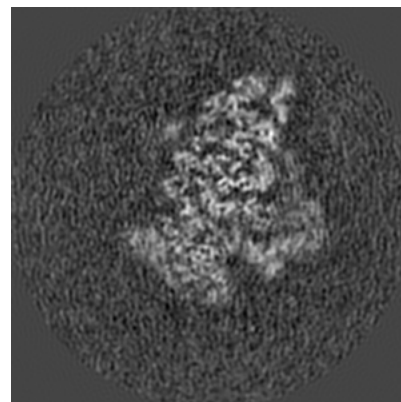
6.2.1 Primary map



X Index: 150

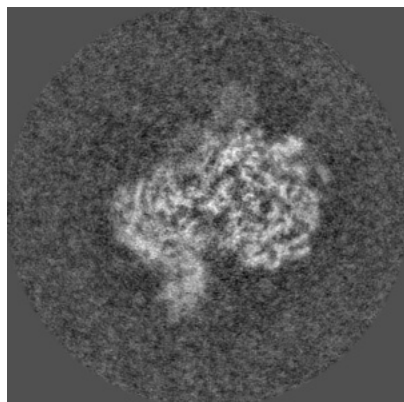


Y Index: 150

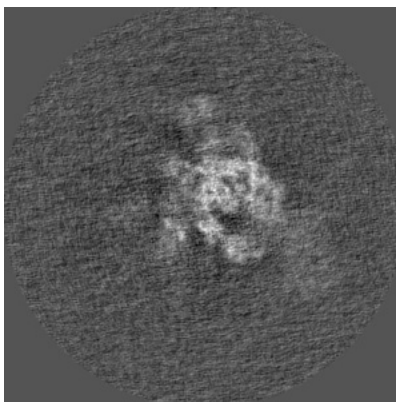


Z Index: 150

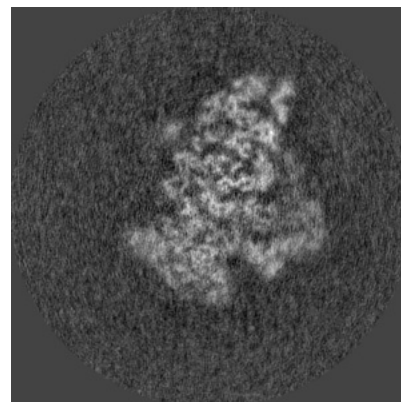
6.2.2 Raw map



X Index: 150



Y Index: 150

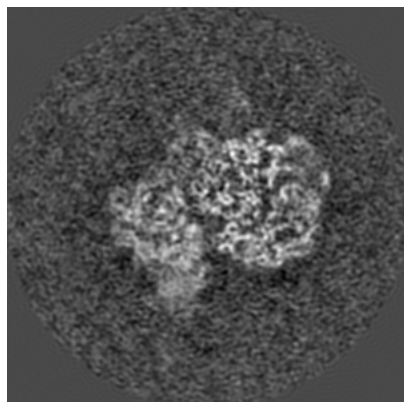


Z Index: 150

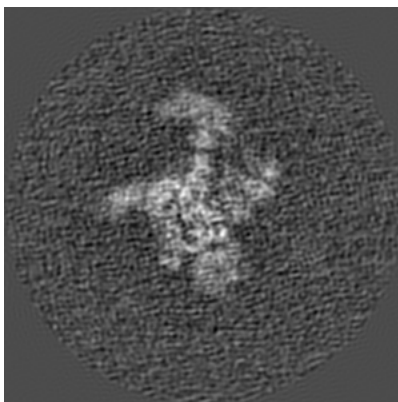
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

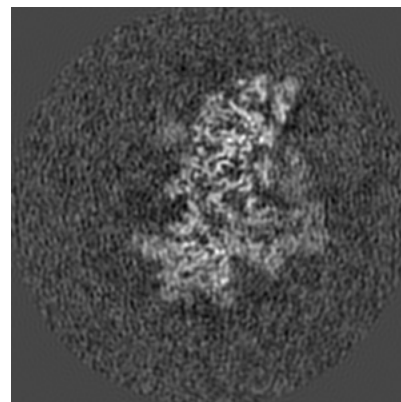
6.3.1 Primary map



X Index: 153

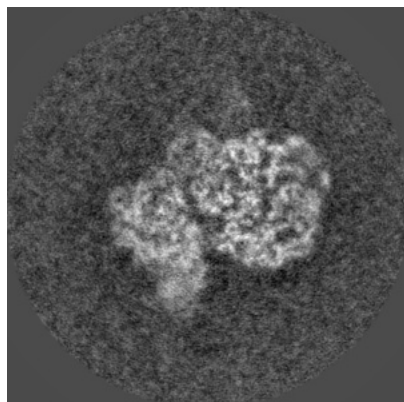


Y Index: 120

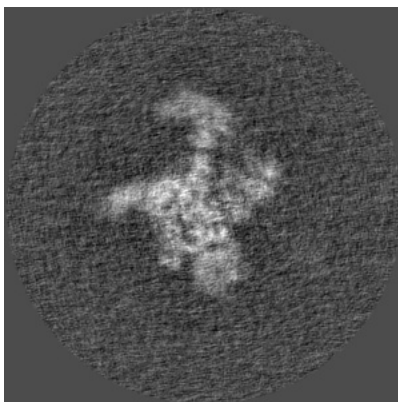


Z Index: 146

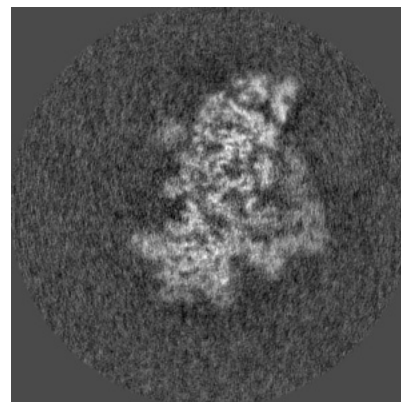
6.3.2 Raw map



X Index: 153



Y Index: 120

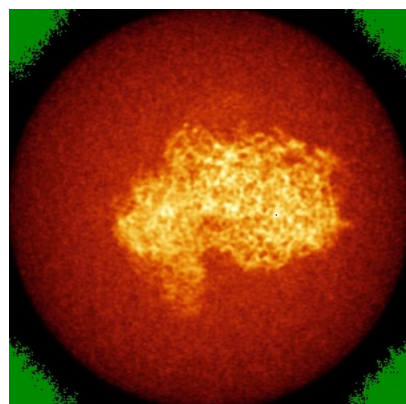


Z Index: 147

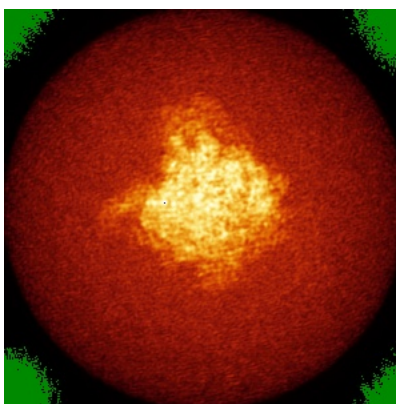
The images above show the largest variance slices of the map in three orthogonal directions.

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

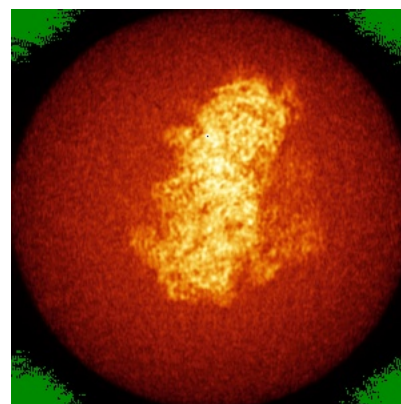
6.4.1 Primary map



X

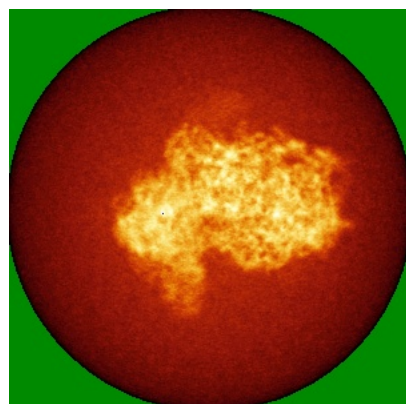


Y

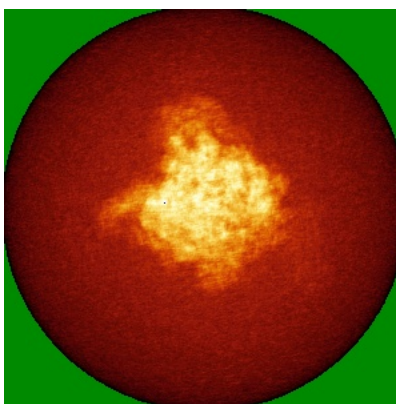


Z

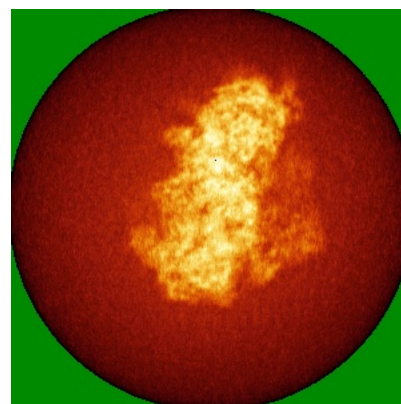
6.4.2 Raw map



X



Y

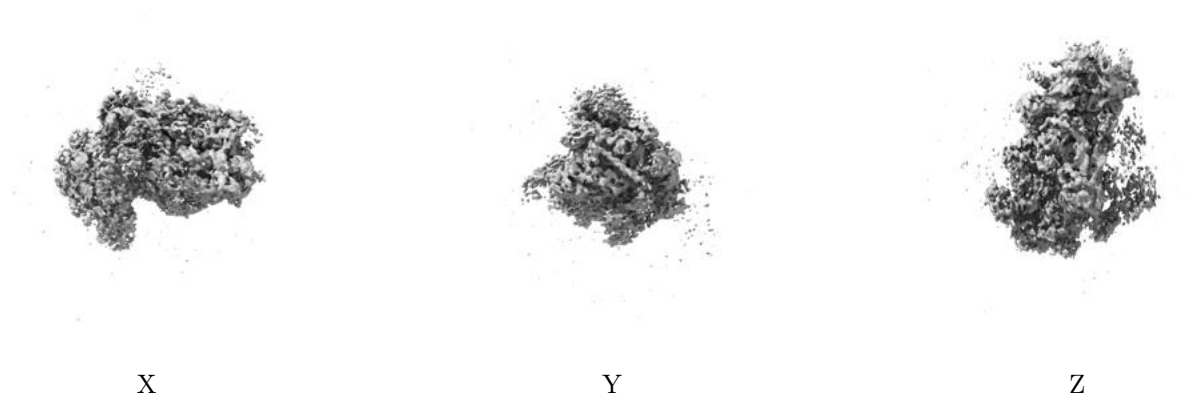


Z

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.

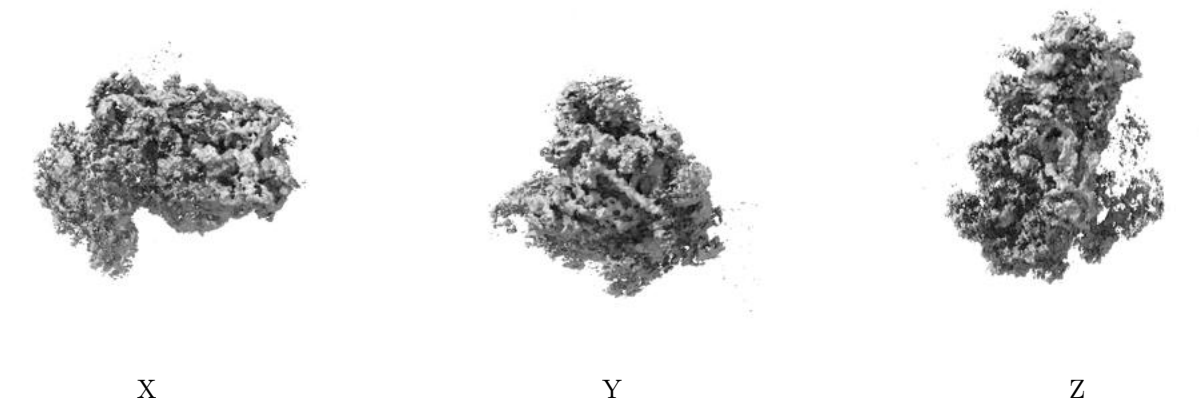
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

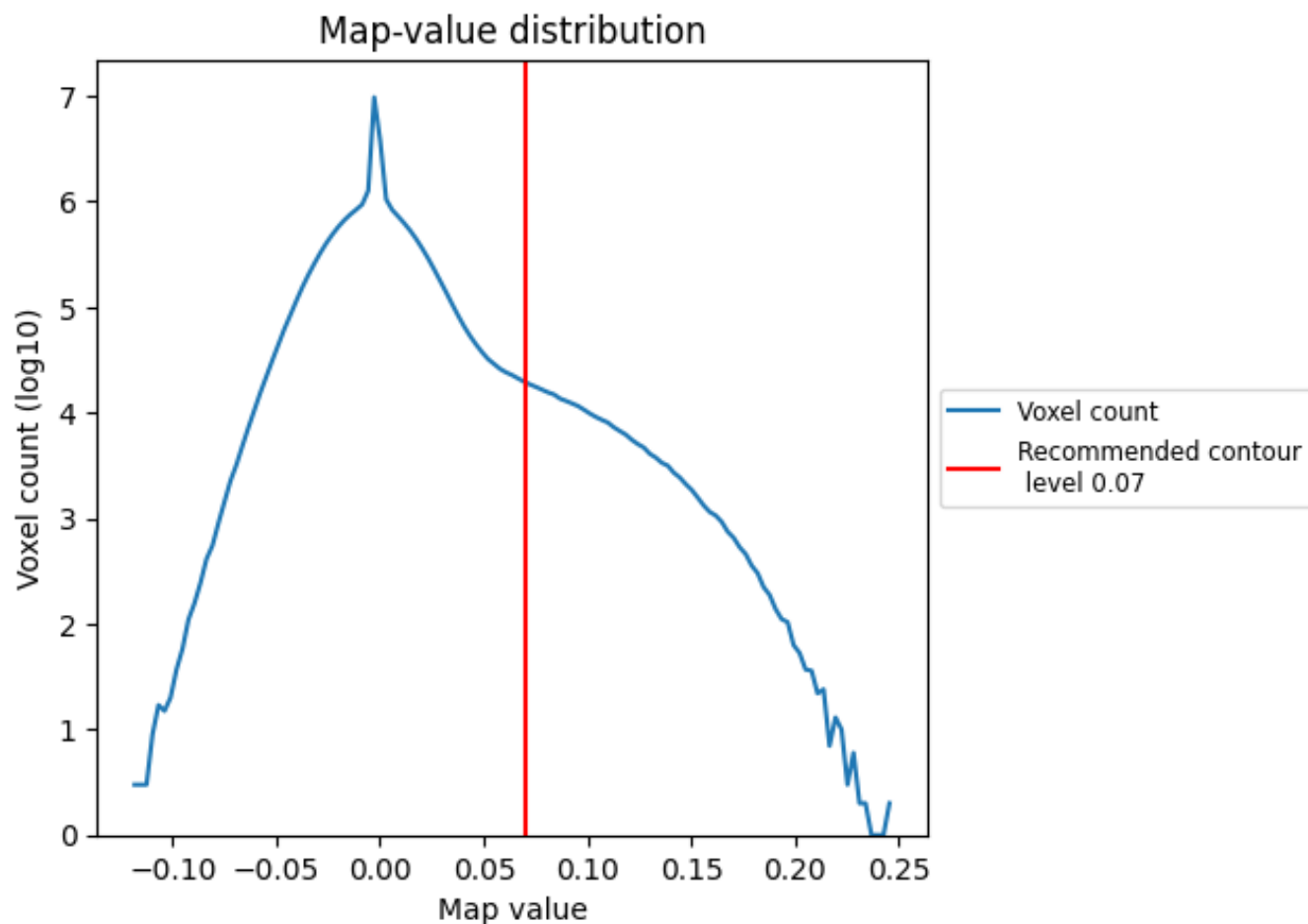
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

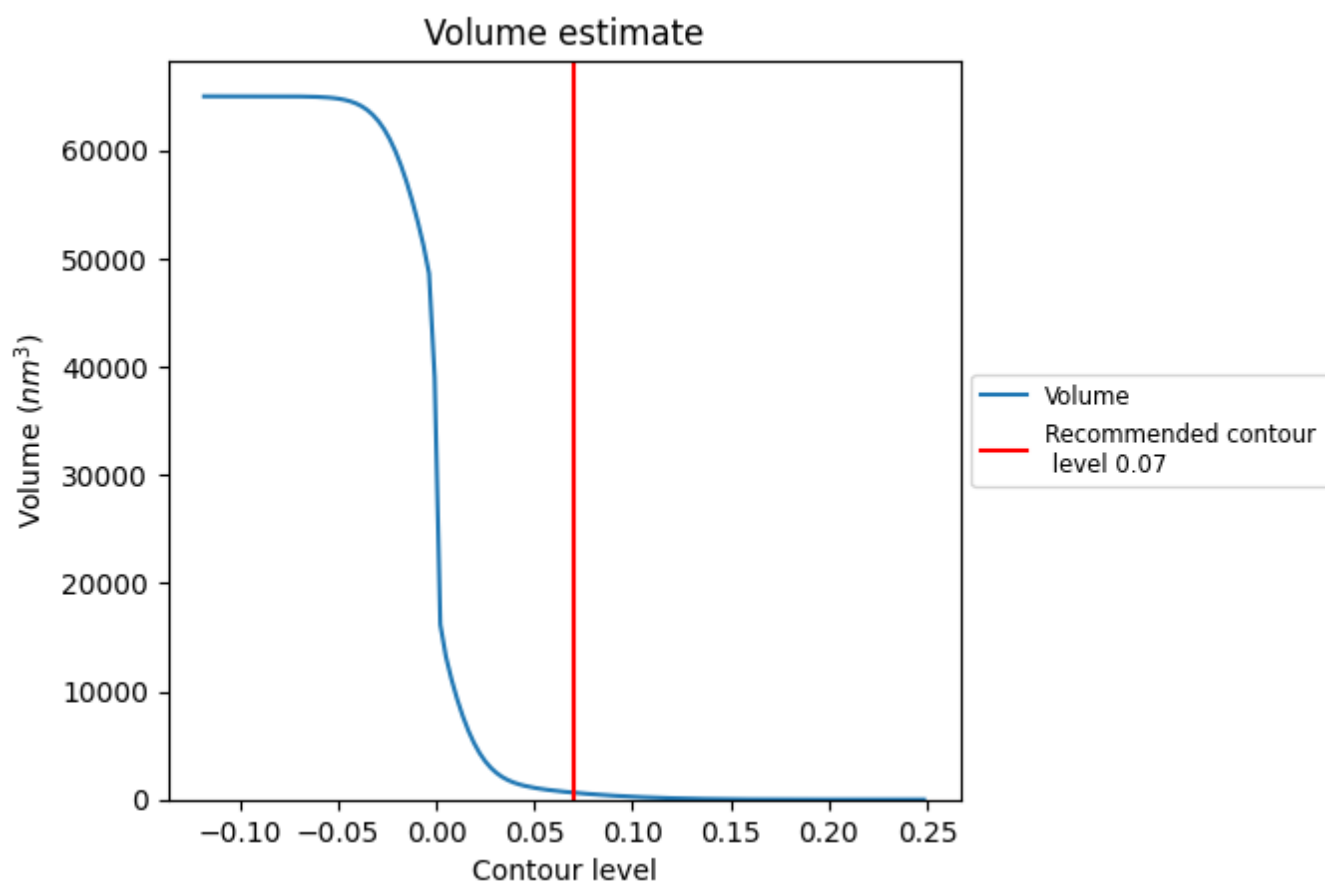
This section contains the results of statistical analysis of the map.

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.

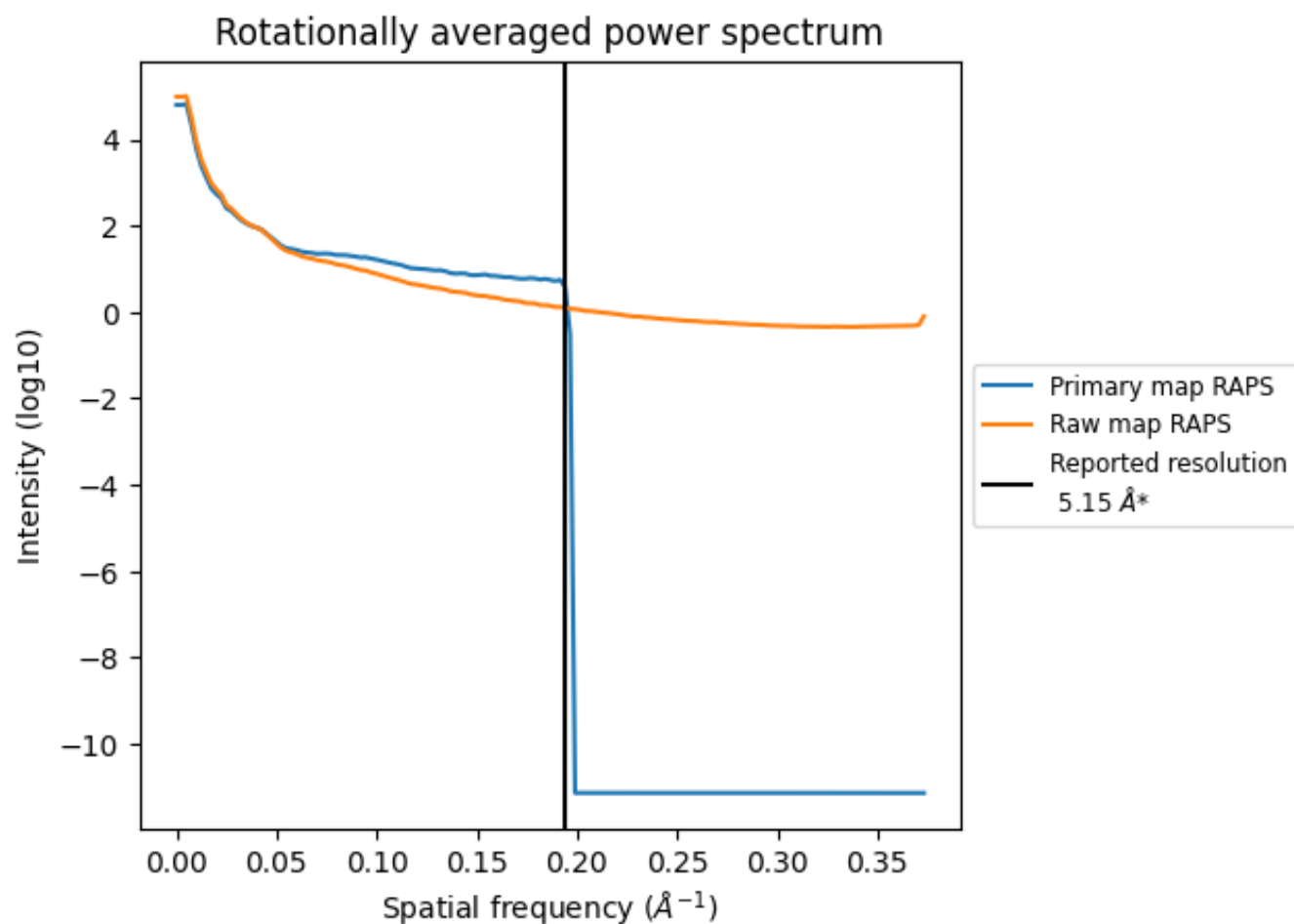
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 638 nm³; this corresponds to an approximate mass of 576 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 ⓘ

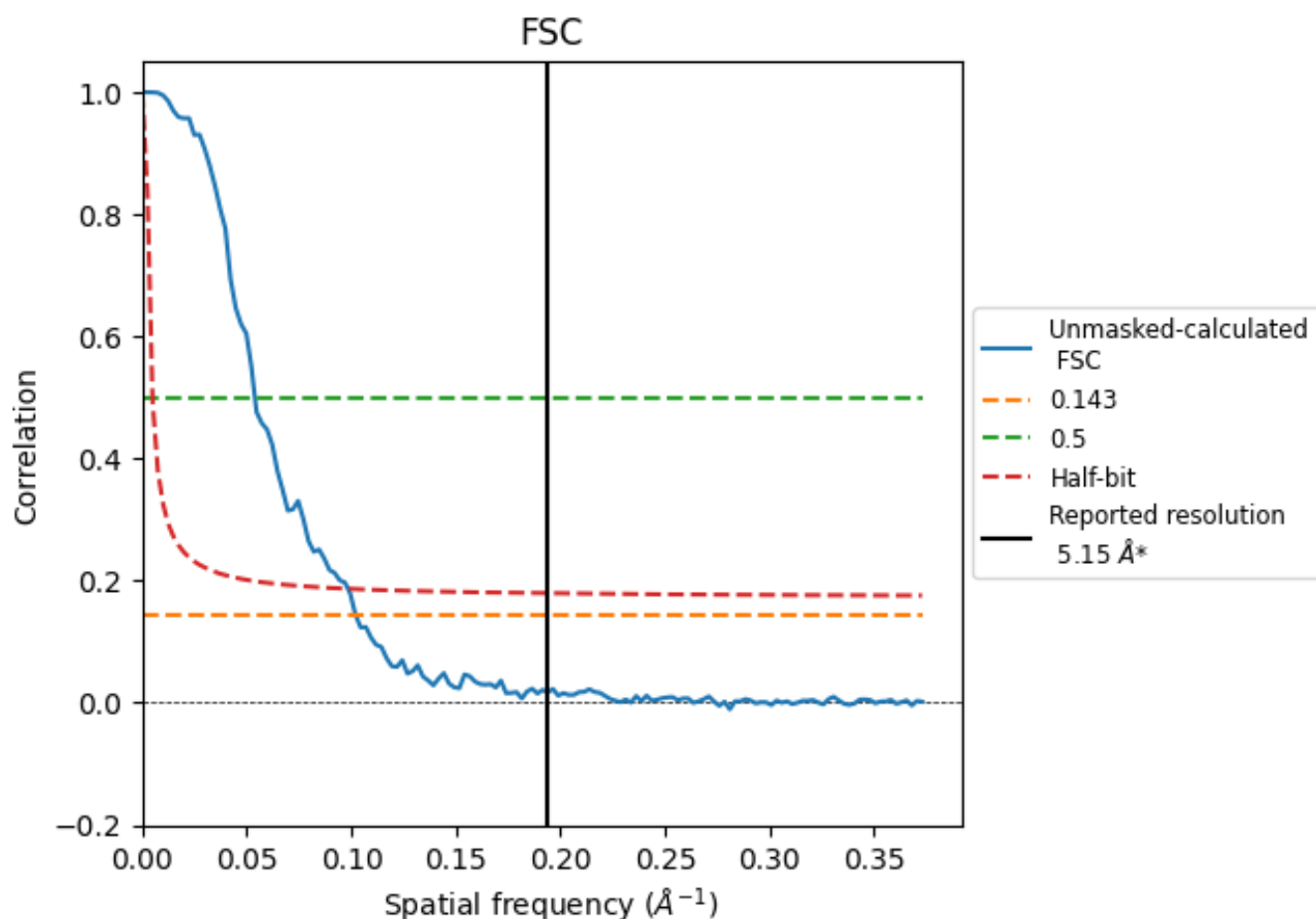


*Reported resolution corresponds to spatial frequency of 0.194 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.194 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

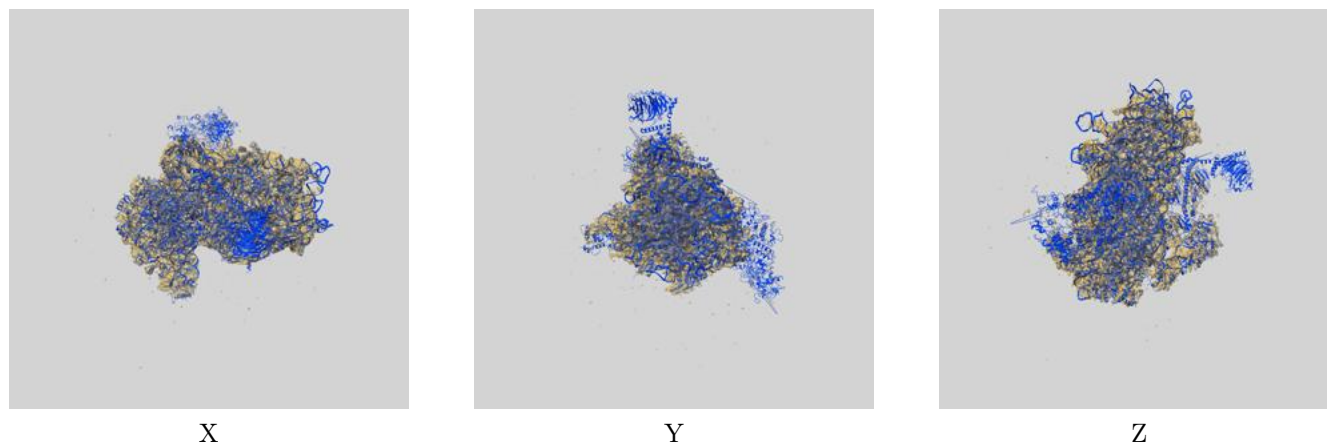
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.15	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.79	18.55	10.16

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.79 differs from the reported value 5.15 by more than 10 %

9 Map-model fit [i](#)

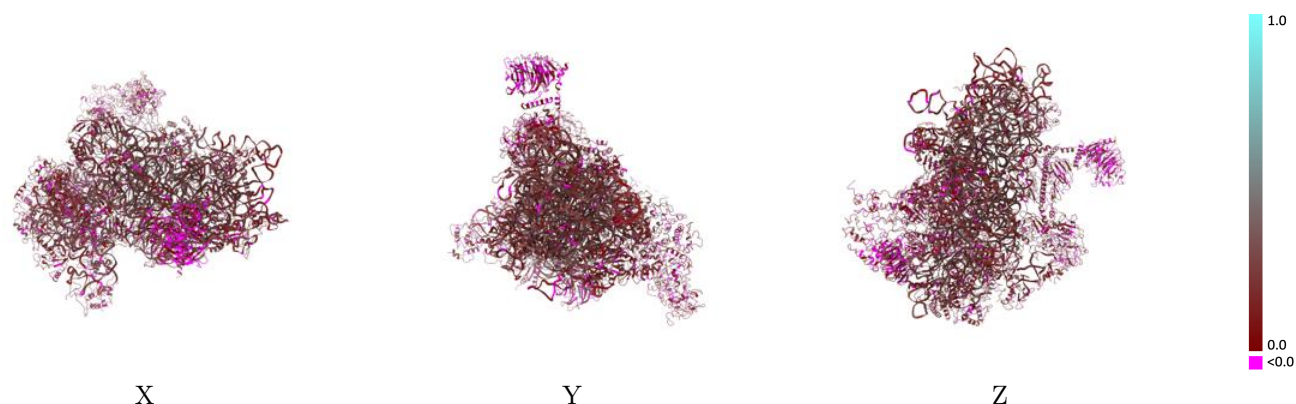
This section contains information regarding the fit between EMDB map EMD-0057 and PDB model 6GSM. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



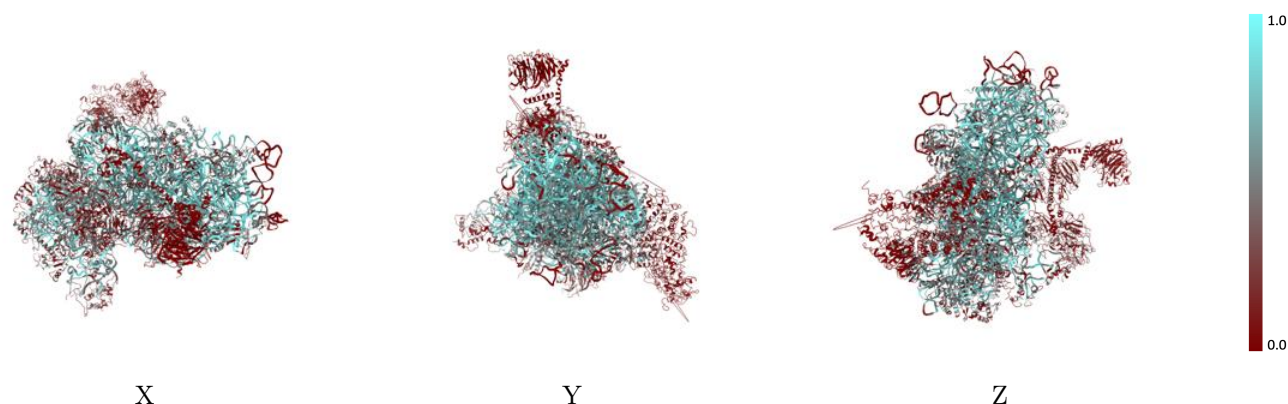
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



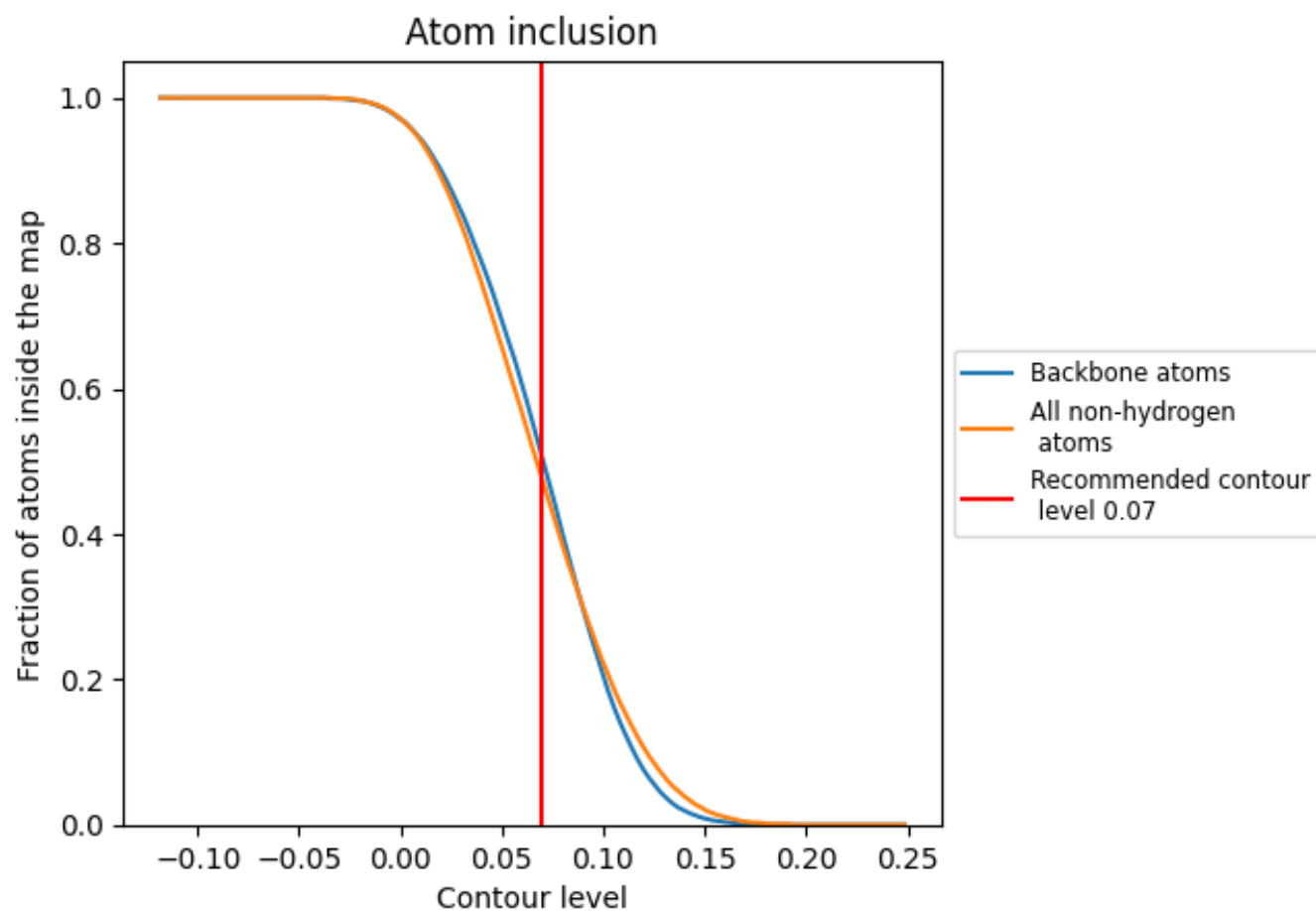
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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 (0.07).

9.4 Atom inclusion [i](#)



At the recommended contour level, 50% of all backbone atoms, 47% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4740	 0.1970
1	 0.6080	 0.1980
2	 0.7540	 0.2370
3	 0.2500	 0.1880
A	 0.4900	 0.2070
B	 0.4830	 0.2200
C	 0.4790	 0.2350
D	 0.3850	 0.2040
E	 0.5390	 0.2180
F	 0.4290	 0.1890
G	 0.4830	 0.1860
H	 0.4360	 0.1970
I	 0.4830	 0.2010
J	 0.5490	 0.2300
K	 0.3610	 0.1570
L	 0.4650	 0.2250
M	 0.1160	 0.1290
N	 0.5540	 0.2160
O	 0.5420	 0.1940
P	 0.3060	 0.1580
Q	 0.4640	 0.1840
R	 0.3890	 0.1990
S	 0.3990	 0.1750
T	 0.5270	 0.1740
U	 0.3340	 0.1690
V	 0.5130	 0.2130
W	 0.5260	 0.2270
X	 0.4330	 0.2240
Y	 0.5620	 0.2130
Z	 0.2250	 0.1680
a	 0.4890	 0.2410
b	 0.4440	 0.2110
c	 0.3300	 0.2070
d	 0.4500	 0.1660
e	 0.3590	 0.2060



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Chain	Atom inclusion	Q-score
f	 0.2300	 0.1300
g	 0.3120	 0.0840
h	 0.1890	 0.1960
i	 0.2450	 0.2080
j	 0.2220	 0.1810
k	 0.1410	 0.1520
l	 0.2150	 0.1960
m	 0.3210	 0.2410
o	 0.0190	 0.1410
p	 0.0490	 0.1440
q	 0.0430	 0.1570
r	 0.0000	 0.0030
s	 0.0000	 0.0140