



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 10:50 PM UTC

PDB ID : 6YLG / pdb_00006ylg
EMDB ID : EMD-10838
Title : Rix1-Rea1 pre-60S particle - 60S core, body 1 (rigid body refinement)
Authors : Kater, L.; Beckmann, R.
Deposited on : 2020-04-07
Resolution : 3.00 Å (reported)
Based on initial models : 3JCT, 6N8J

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:

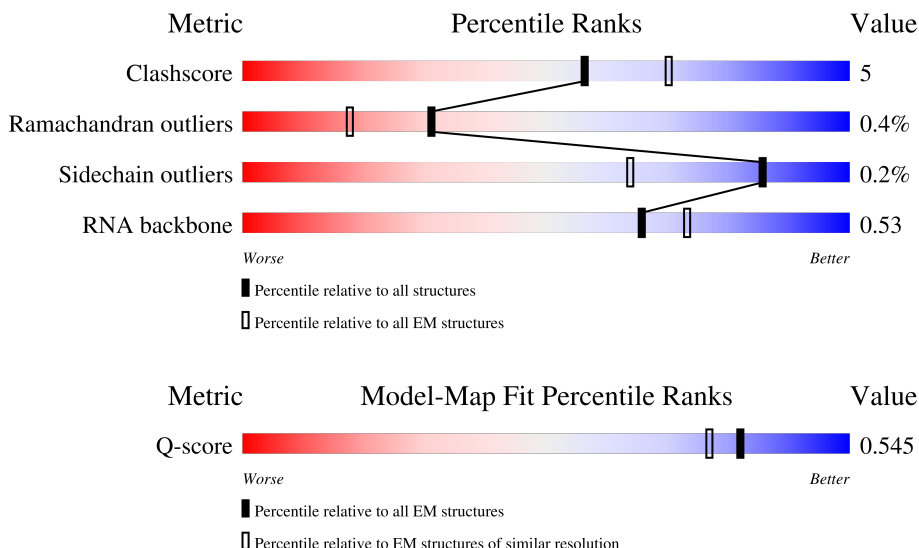
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.00 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.



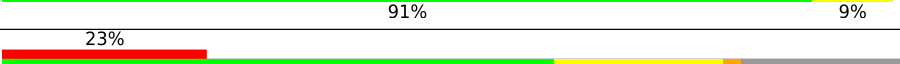
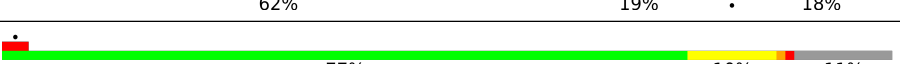
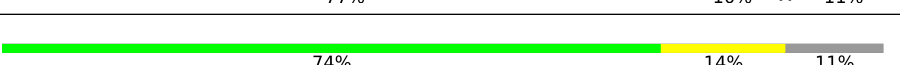
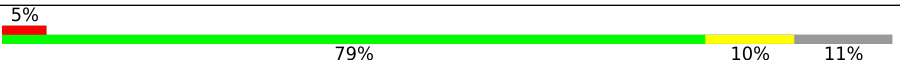
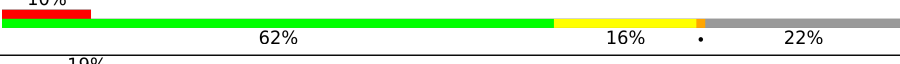
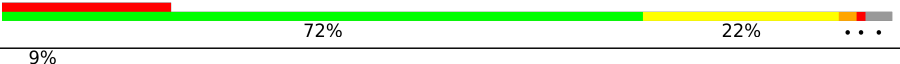
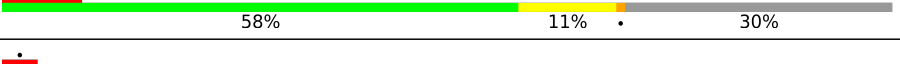
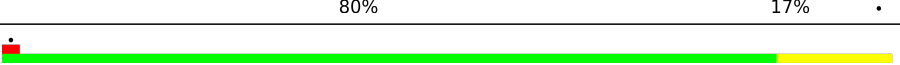
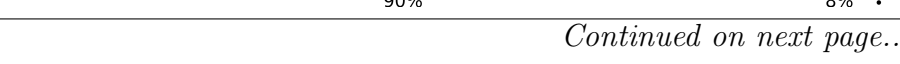
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	3396	
2	2	158	
3	3	121	

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Mol	Chain	Length	Quality of chain
4	4	593	
5	5	120	
6	A	254	
7	B	387	
8	C	362	
9	D	297	
10	E	176	
11	F	244	
12	G	256	
13	H	191	
14	I	166	
15	J	174	
16	K	334	
17	L	199	
18	M	138	
19	N	204	
20	O	199	
21	P	184	
22	Q	186	
23	R	189	
24	S	172	
25	T	160	
26	U	121	
27	V	137	
28	W	236	

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Mol	Chain	Length	Quality of chain
29	X	142	
30	Y	127	
31	Z	136	
32	a	149	
33	b	647	
34	c	175	
35	d	113	
36	e	130	
37	f	107	
38	g	121	
39	h	120	
40	i	100	
41	j	88	
42	k	78	
43	l	51	
44	m	486	
45	n	105	
46	o	217	
47	p	92	
48	q	165	
49	r	261	
50	s	520	
51	t	767	
52	u	199	
53	x	515	

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Mol	Chain	Length	Quality of chain
54	y	245	12% 65% 28% 6%
55	z	106	12% 64% 8% 27%

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 147190 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 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	3039	Total	C	N	O	P	0	0
			65028	29041	11740	21208	3039		

- Molecule 2 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	154	Total	C	N	O	P	0	0
			3273	1464	576	1079	154		

- Molecule 3 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	117	Total	C	N	O	P	0	0
			2494	1114	446	817	117		

- Molecule 4 is a protein called Probable metalloprotease ARX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	509	Total	C	N	O	S	0	0
			3945	2503	673	754	15		

- Molecule 5 is a protein called rRNA-processing protein CGR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	78	Total	C	N	O	S	0	0
			681	419	140	119	3		

- Molecule 6 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	245	Total	C	N	O	S	0	0
			1863	1162	376	324	1		

- Molecule 7 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	386	Total	C	N	O	S	0	0
			3081	1956	584	533	8		

- Molecule 8 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	361	Total	C	N	O	S	0	0
			2749	1730	522	494	3		

- Molecule 9 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	243	Total	C	N	O	S	0	0
			1969	1250	344	373	2		

- Molecule 10 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	156	Total	C	N	O	S	0	0
			1239	800	222	216	1		

- Molecule 11 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	216	Total	C	N	O	S	0	0
			1744	1127	317	299	1		

- Molecule 12 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	228	Total	C	N	O	S	0	0
			1784	1142	320	319	3		

- Molecule 13 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	187	Total	C	N	O	S	0	0
			1486	944	270	268	4		

- Molecule 14 is a protein called Bud site selection protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	130	Total	C	N	O	S	0	0
			1051	657	194	197	3		

- Molecule 15 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	168	Total	C	N	O	S	0	0
			1344	841	251	248	4		

- Molecule 16 is a protein called Pre-rRNA-processing protein IPI1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	234	Total	C	N	O	S	0	0
			1875	1203	331	333	8		

- Molecule 17 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	181	Total	C	N	O	S	0	0
			1456	907	301	248			

- Molecule 18 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	134	Total	C	N	O	S	0	0
			1040	666	196	176	2		

- Molecule 19 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	N	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 20 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	O	197	Total	C	N	O	S	0	0
			1555	1003	289	262	1		

- Molecule 21 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	P	171	Total	C	N	O	0	0
			1360	845	272	243		

- Molecule 22 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Q	144	Total	C	N	O	S	0	0
			1110	704	213	192	1		

- Molecule 23 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	R	151	Total	C	N	O	0	0
			1219	757	258	204		

- Molecule 24 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	S	171	Total	C	N	O	S	0	0
			1437	925	266	243	3		

- Molecule 25 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	T	124	Total	C	N	O	S	0	0
			983	619	188	173	3		

- Molecule 26 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	U	101	Total	C	N	O	0	0
			800	518	131	151		

- Molecule 27 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	V	134	Total	C	N	O	S	0	0
			993	623	187	176	7		

- Molecule 28 is a protein called Ribosome assembly factor MRT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	W	233	Total	C	N	O	S	0	0
			1877	1189	322	361	5		

- Molecule 29 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	X	140	Total	C	N	O	S	0	0
			1092	699	195	196	2		

- Molecule 30 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Y	125	Total	C	N	O		0	0
			984	620	191	173			

- Molecule 31 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Z	135	Total	C	N	O		0	0
			1092	710	202	180			

- Molecule 32 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	93	Total	C	N	O	S	0	0
			735	479	130	125	1		

- Molecule 33 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	613	Total	C	N	O	S	0	0
			4953	3110	892	926	25		

- Molecule 34 is a protein called Ribosome biogenesis protein ALB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	c	109	Total	C	N	O		0	0
			872	543	171	158			

- Molecule 35 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	d	105	Total	C	N	O	S	0	0
			856	544	163	148	1		

- Molecule 36 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	e	127	Total	C	N	O	S	0	0
			1020	647	205	167	1		

- Molecule 37 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 38 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	g	107	Total	C	N	O	S	0	0
			846	525	173	144	4		

- Molecule 39 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	h	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 40 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	i	96	Total	C	N	O	S	0	0
			743	465	148	128	2		

- Molecule 41 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	j	84	Total	C	N	O	S	0	0
			665	405	145	110	5		

- Molecule 42 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	k	77	Total	C	N	O	0	0
			612	391	115	106		

- Molecule 43 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	l	49	Total	C	N	O	S	0	0
			428	266	96	64	2		

- Molecule 44 is a protein called Nucleolar GTP-binding protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	m	439	Total	C	N	O	S	0	0
			3546	2249	647	641	9		

- Molecule 45 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	n	97	Total	C	N	O	S	0	0
			743	479	124	139	1		

- Molecule 46 is a protein called 60S ribosomal protein L1-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	o	177	Total	C	N	O	0	0
			877	523	177	177		

- Molecule 47 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	p	89	Total	C	N	O	S	0	0
			680	421	136	117	6		

- Molecule 48 is a protein called 60S ribosomal protein L12-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	q	126	Total	C	N	O	S	0	0
			961	606	171	182	2		

- Molecule 49 is a protein called Ribosome biogenesis protein NSA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	r	225	Total	C	N	O	S	0	0
			1818	1152	345	314	7		

- Molecule 50 is a protein called Nuclear GTP-binding protein NUG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	s	56	Total	C	N	O	S	0	0
			463	291	94	77	1		

- Molecule 51 is a protein called Protein SDA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	t	431	Total	C	N	O	S	0	0
			3395	2156	587	629	23		

- Molecule 52 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	u	148	Total	C	N	O	S	0	0
			1247	783	250	205	9		

- Molecule 53 is a protein called Ribosome assembly protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	x	388	Total	C	N	O	S	0	0
			3033	1900	549	564	20		

- Molecule 54 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	y	243	Total	C	N	O	S	0	0
			1841	1141	318	376	6		

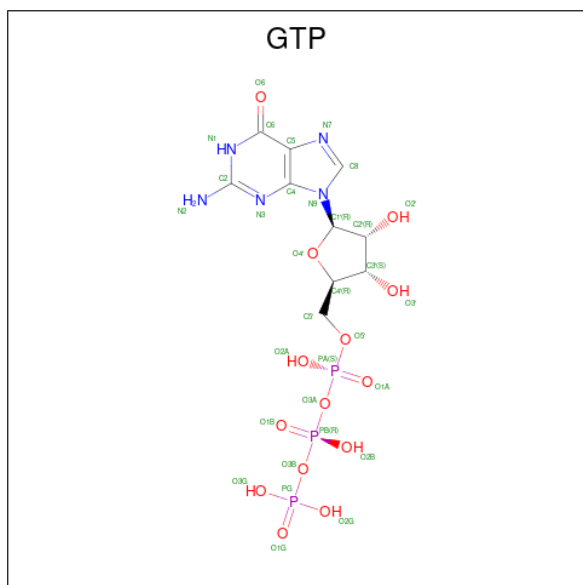
- Molecule 55 is a protein called UPF0642 protein YBL028C.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	z	77	Total	C	N	O	S	0	0
			643	403	130	109	1		

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
56	I	1	Total	Zn	0
			1	1	
56	j	1	Total	Zn	0
			1	1	
56	p	1	Total	Zn	0
			1	1	
56	u	1	Total	Zn	0
			1	1	

- Molecule 57 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
57	b	1	Total	C	N	O	P	0
			32	10	5	14	3	
57	m	1	Total	C	N	O	P	0
			32	10	5	14	3	

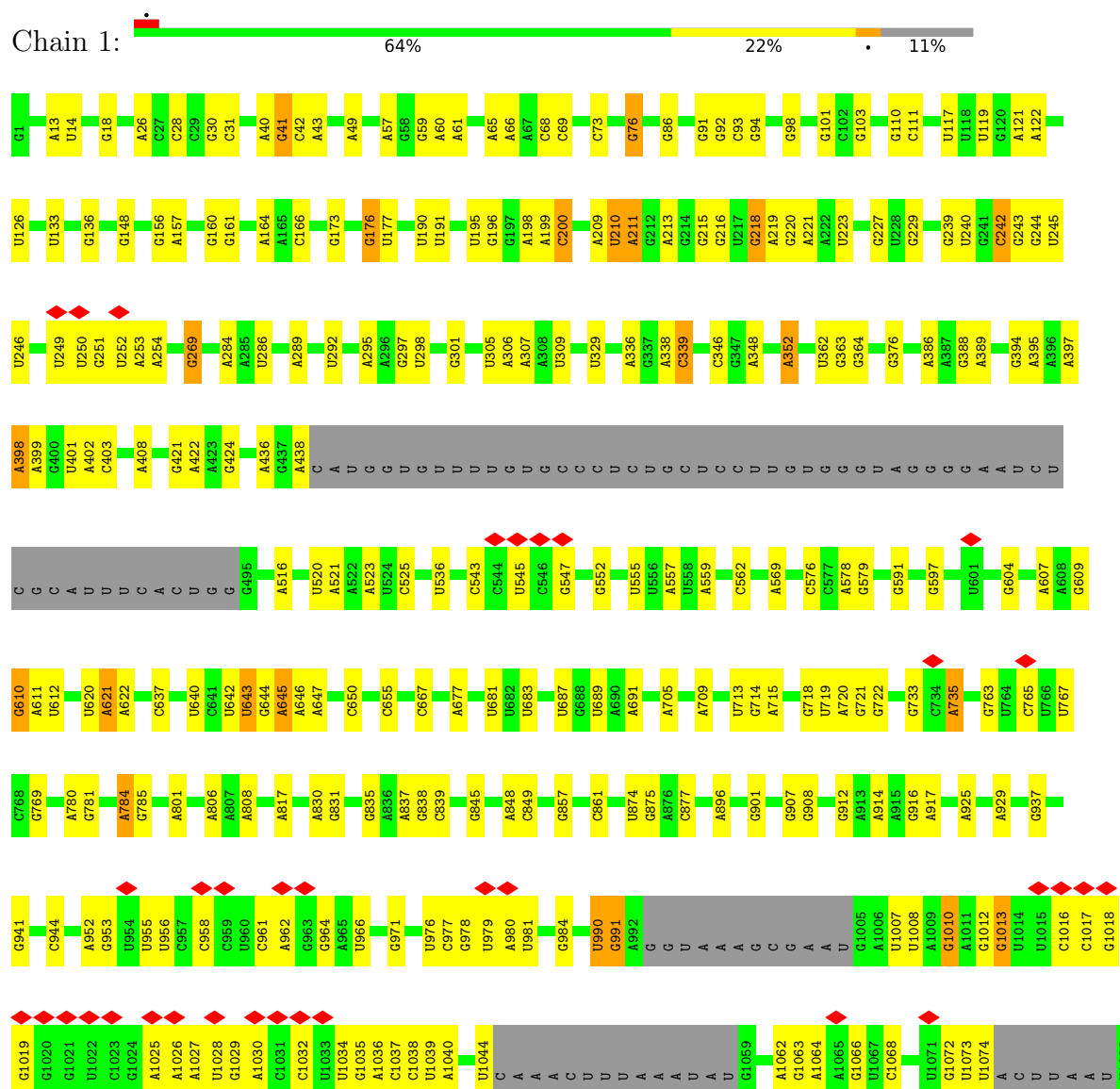
- Molecule 58 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
58	b	1	Total	Mg	0
			1	1	
58	m	1	Total	Mg	0
			1	1	

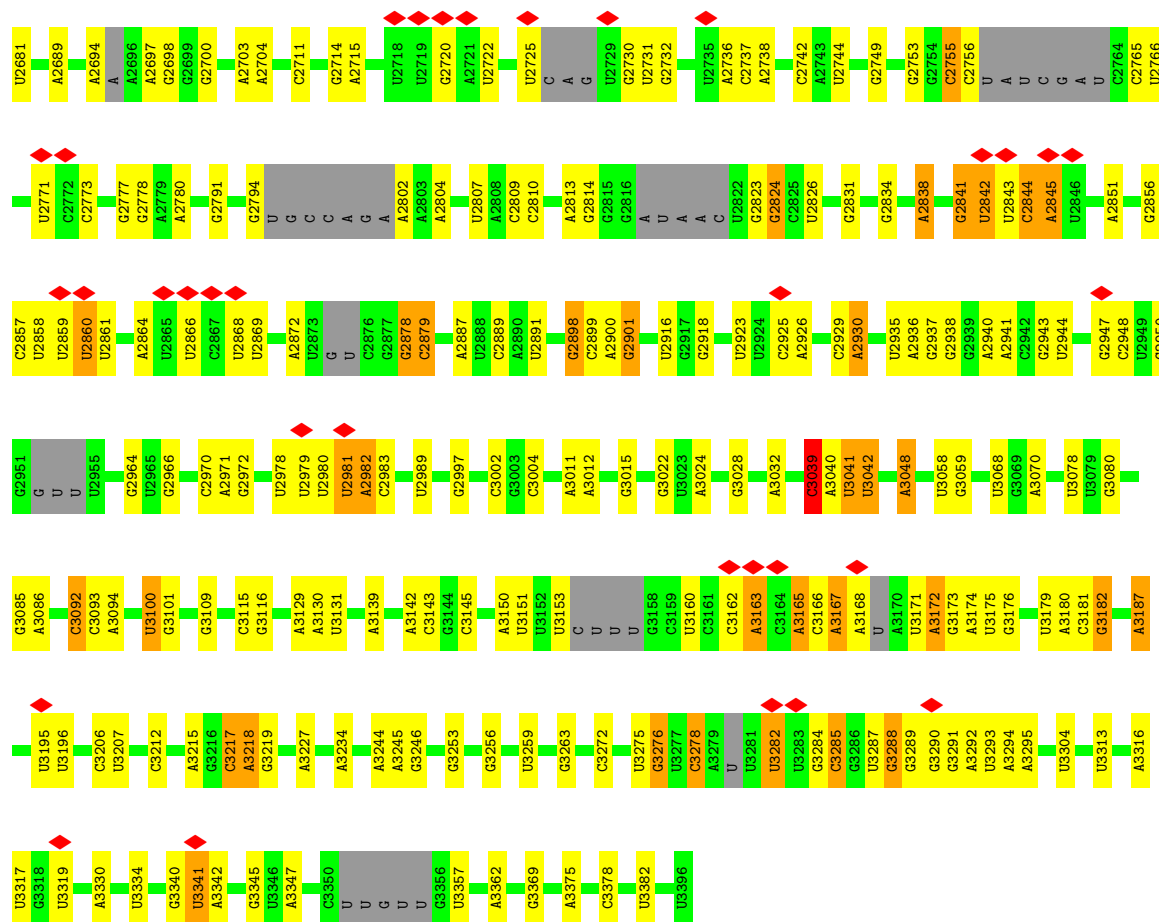
3 Residue-property plots

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

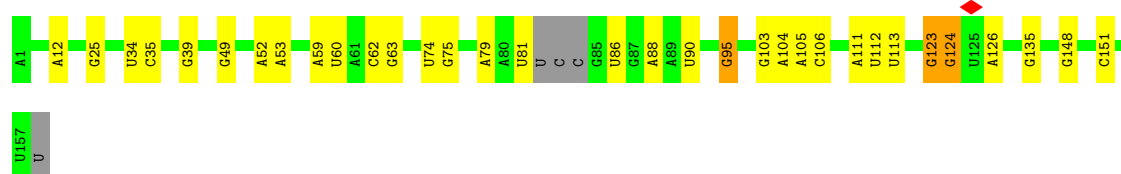
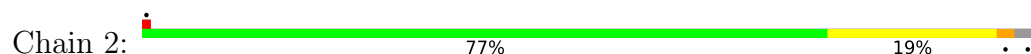
• Molecule 1: 25S rRNA



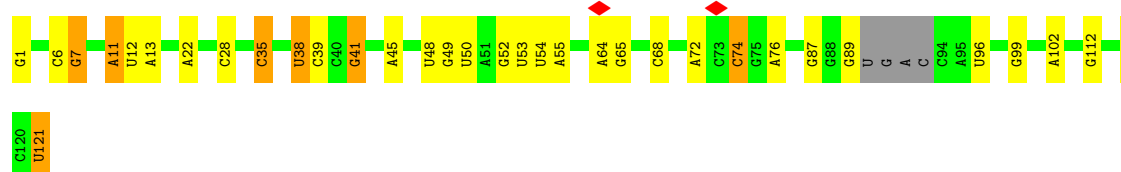




• Molecule 2: 5.8S rRNA

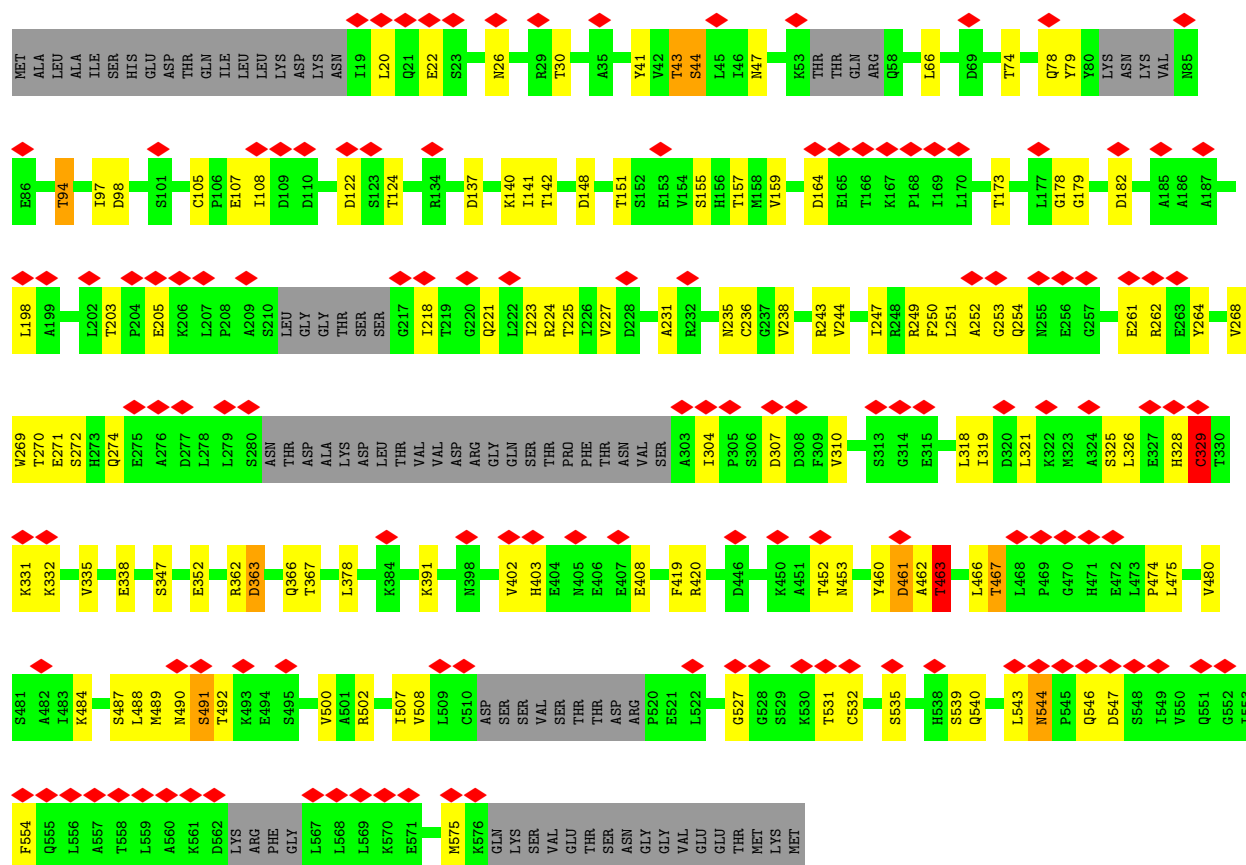


• Molecule 3: 5S rRNA

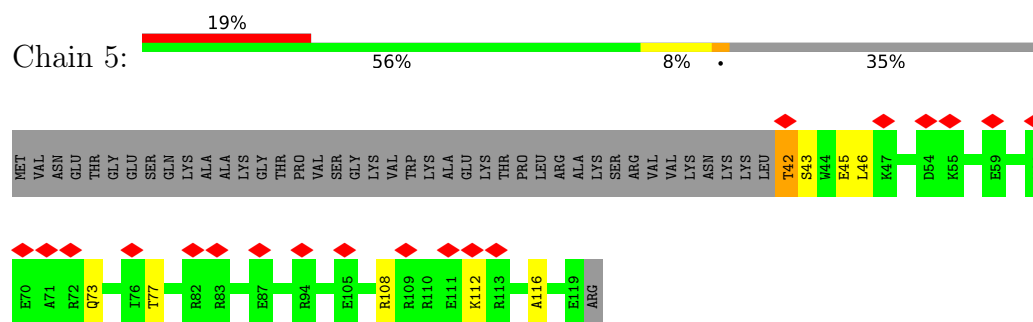


• Molecule 4: Probable metalloprotease ARX1

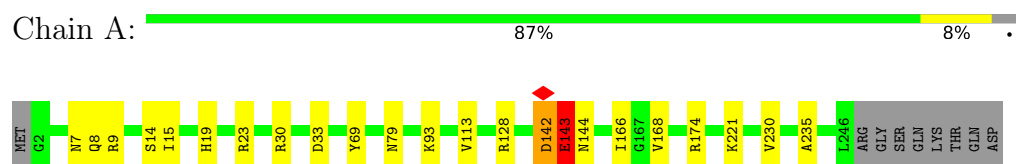




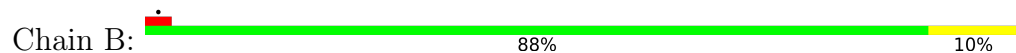
• Molecule 5: rRNA-processing protein CGR1

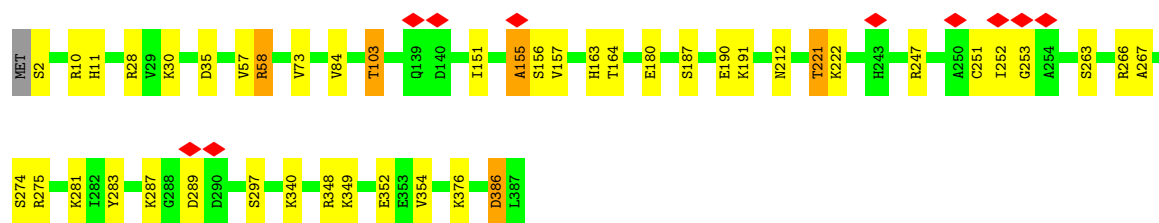


• Molecule 6: 60S ribosomal protein L2-A

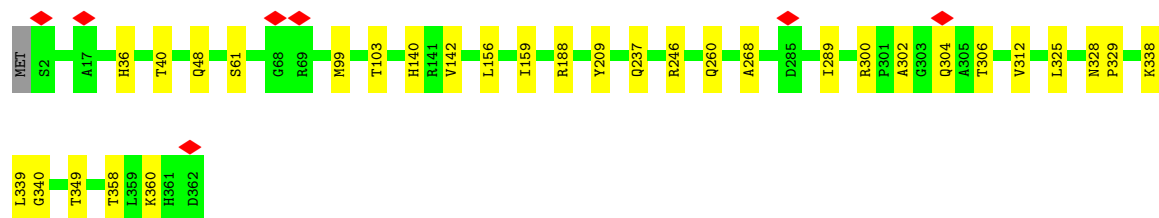


• Molecule 7: 60S ribosomal protein L3

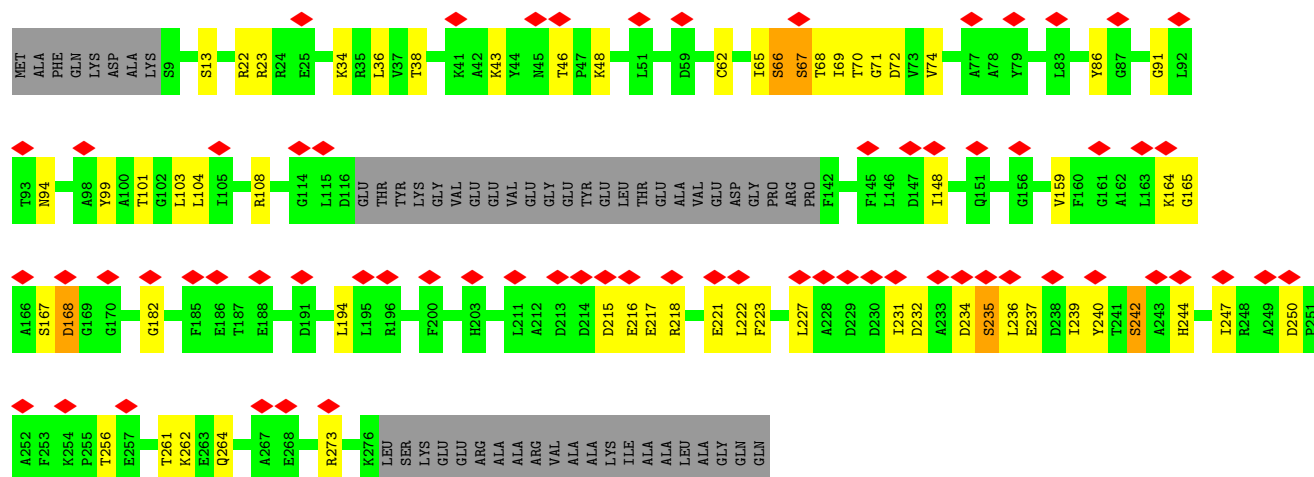




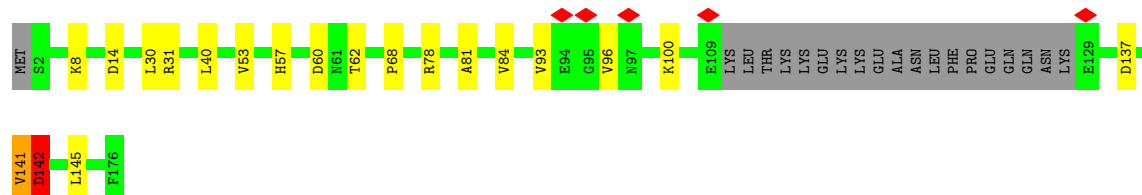
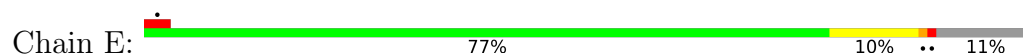
• Molecule 8: 60S ribosomal protein L4-A



• Molecule 9: 60S ribosomal protein L5

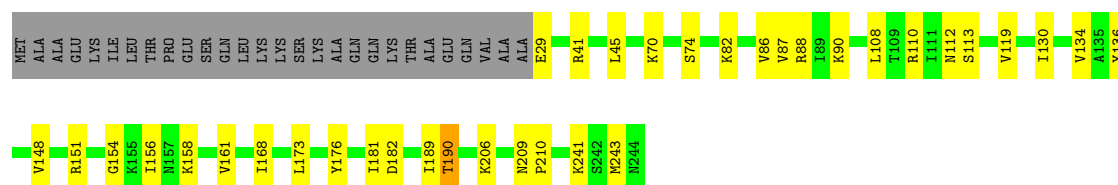


• Molecule 10: 60S ribosomal protein L6-A



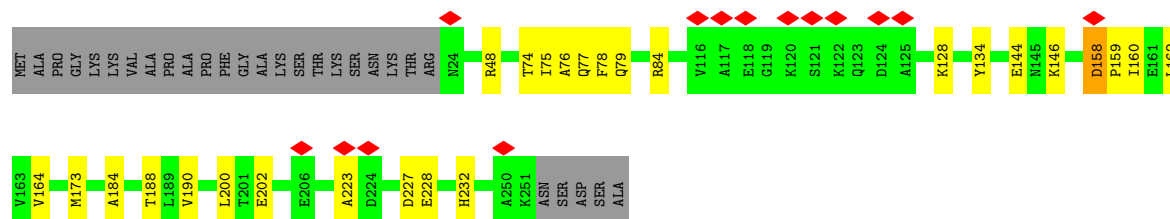
• Molecule 11: 60S ribosomal protein L7-A

Chain F: 



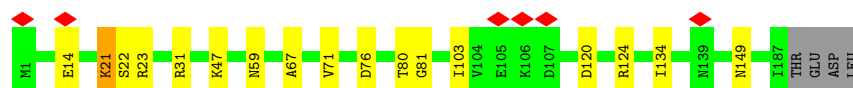
- Molecule 12: 60S ribosomal protein L8-A

Chain G: 



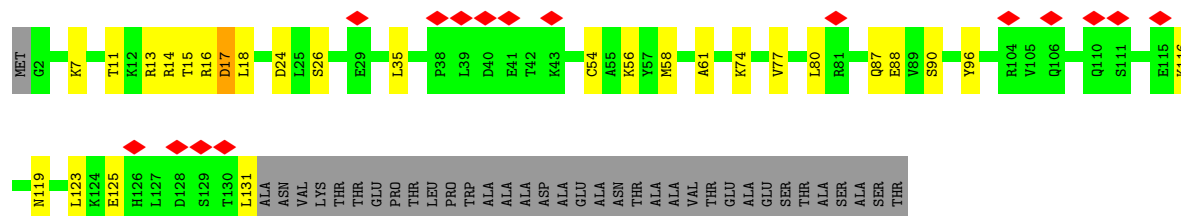
- Molecule 13: 60S ribosomal protein L9-A

Chain H: 



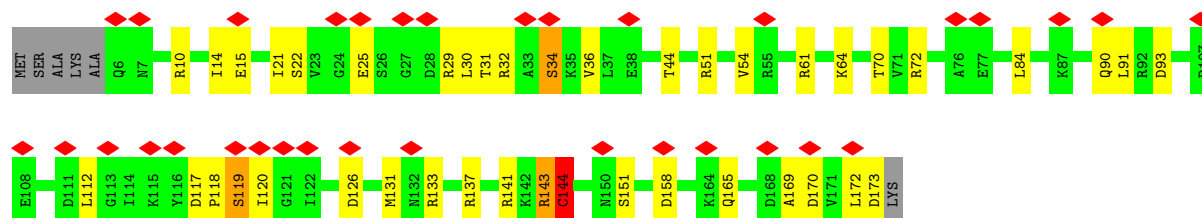
- Molecule 14: Bud site selection protein 20

Chain I: 

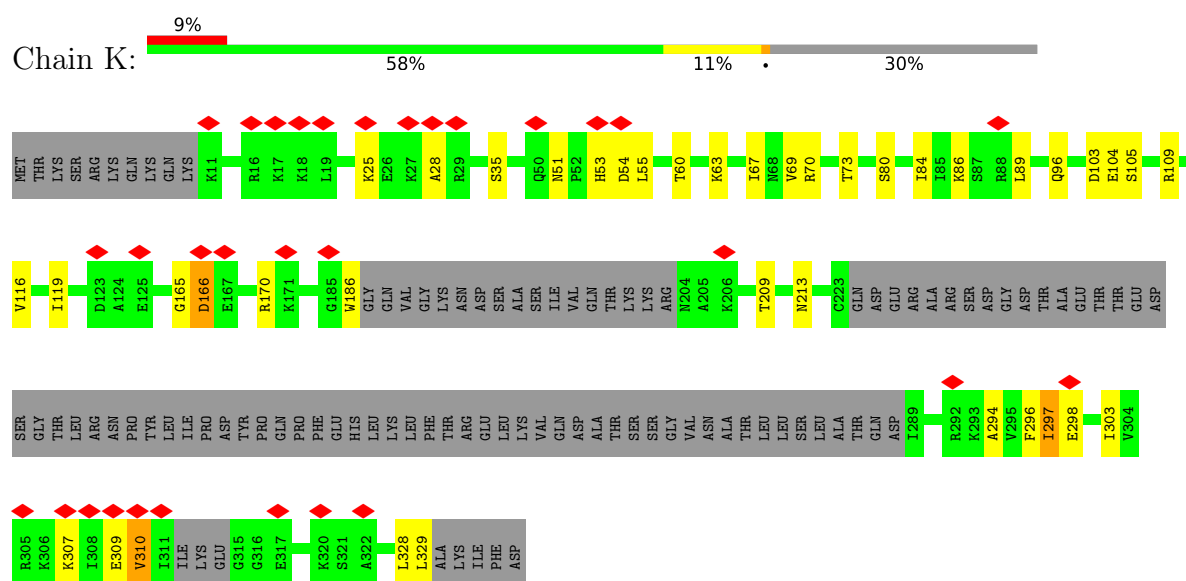


- Molecule 15: 60S ribosomal protein L11-A

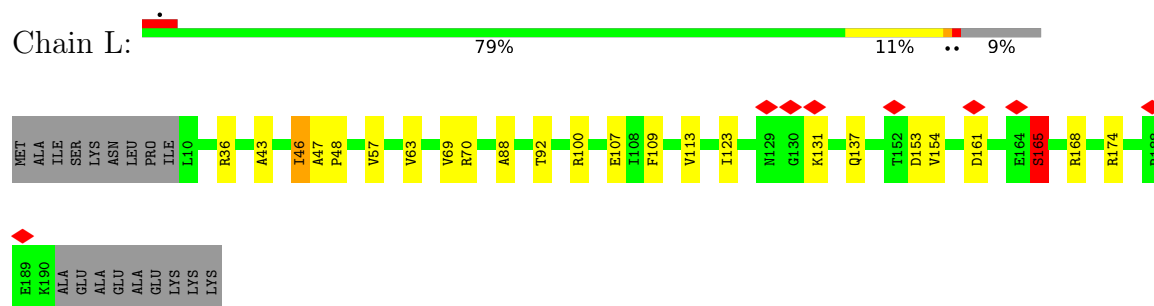
Chain J: 



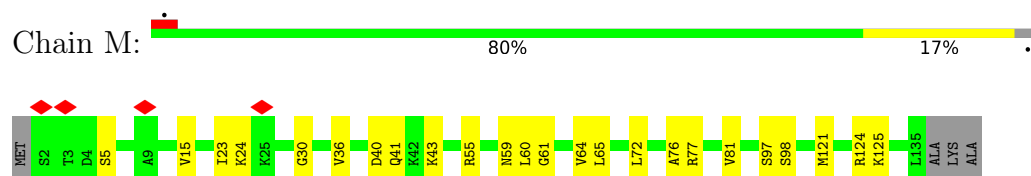
- Molecule 16: Pre-rRNA-processing protein IPI1



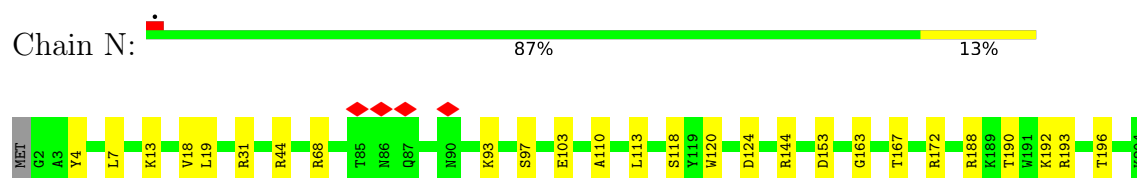
• Molecule 17: 60S ribosomal protein L13-A



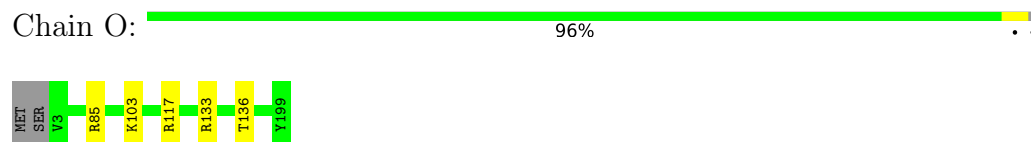
• Molecule 18: 60S ribosomal protein L14-A



• Molecule 19: 60S ribosomal protein L15-A

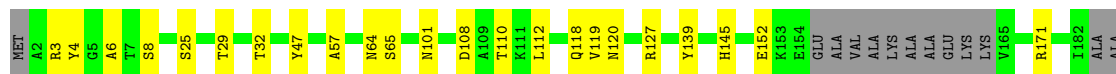


• Molecule 20: 60S ribosomal protein L16-A



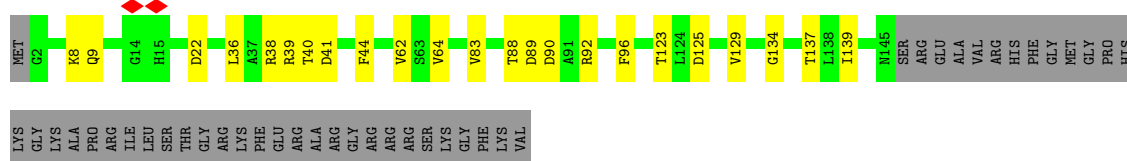
- Molecule 21: 60S ribosomal protein L17-A

Chain P:  80% 12% 7%



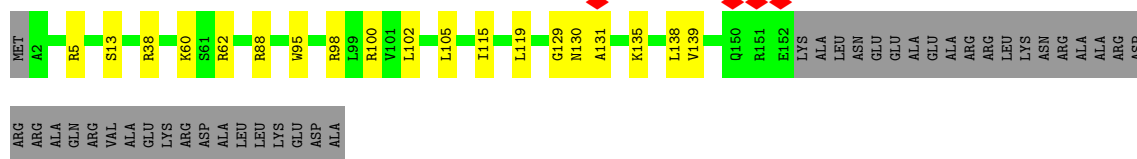
- Molecule 22: 60S ribosomal protein L18-A

Chain Q:  65% 12% 23%



- Molecule 23: 60S ribosomal protein L19-A

Chain R:  70% 10% 20%



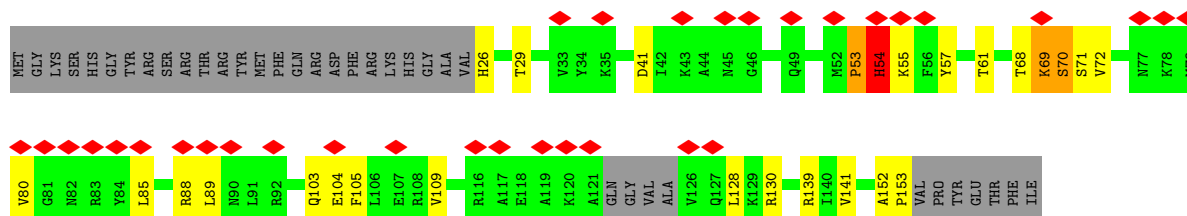
- Molecule 24: 60S ribosomal protein L20-A

Chain S:  5% 81% 17% ...



- Molecule 25: 60S ribosomal protein L21-A

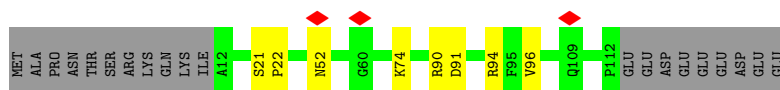
Chain T:  21% 61% 14% .. 22%



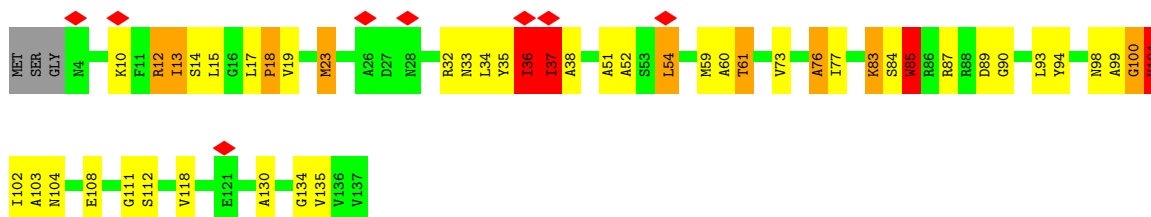
- Molecule 26: 60S ribosomal protein L22-A

Chain U:  77% 7% 17%





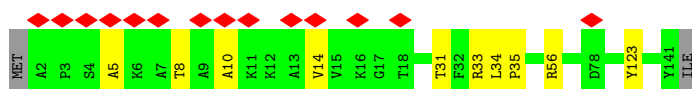
- Molecule 27: 60S ribosomal protein L23-A



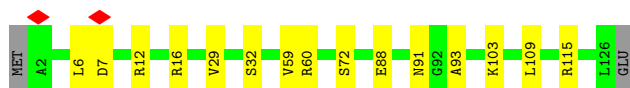
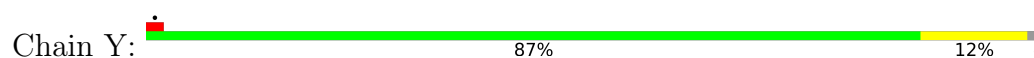
- Molecule 28: Ribosome assembly factor MRT4



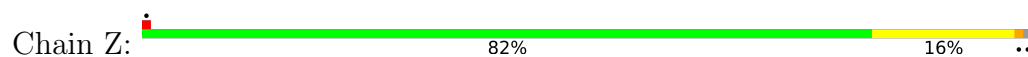
- Molecule 29: 60S ribosomal protein L25



- Molecule 30: 60S ribosomal protein L26-A

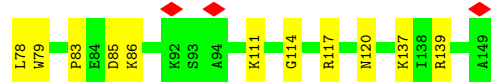
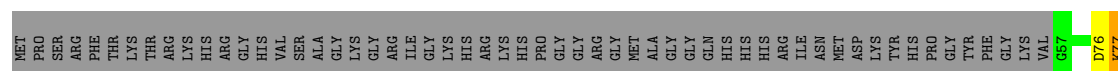


- Molecule 31: 60S ribosomal protein L27-A

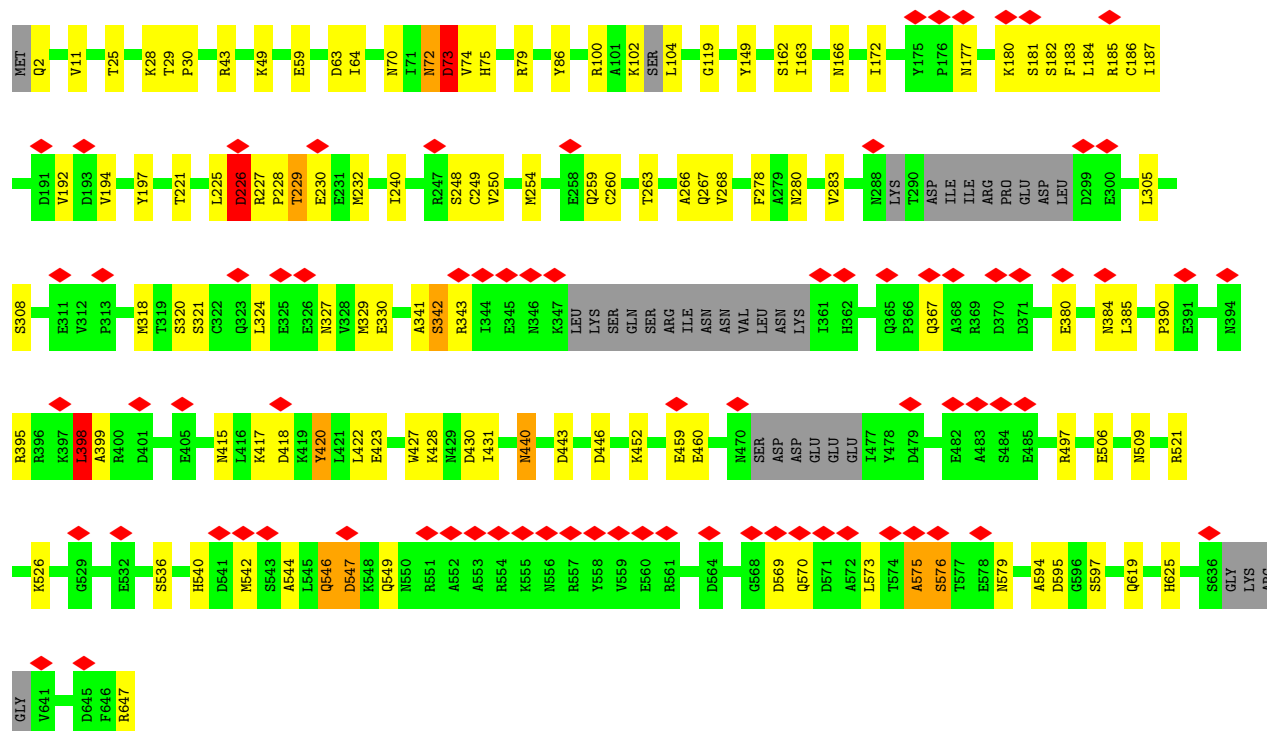
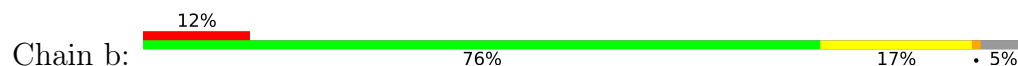


- Molecule 32: 60S ribosomal protein L28

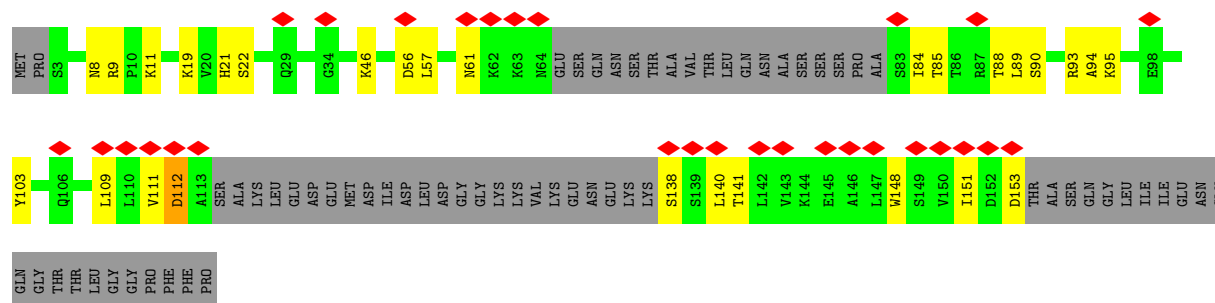




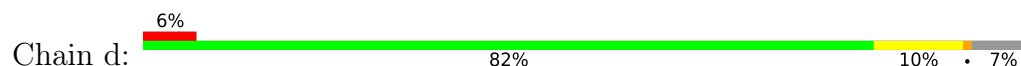
• Molecule 33: Nucleolar GTP-binding protein 1



• Molecule 34: Ribosome biogenesis protein ALB1

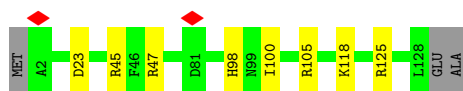
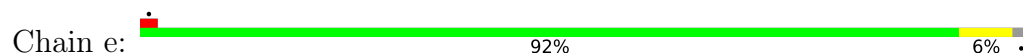


• Molecule 35: 60S ribosomal protein L31-A

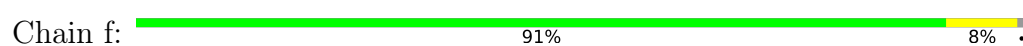




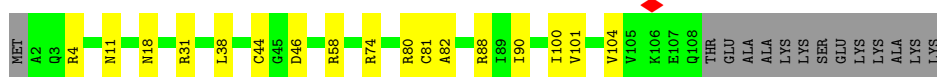
- Molecule 36: 60S ribosomal protein L32



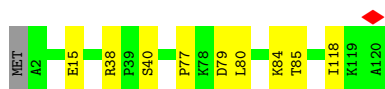
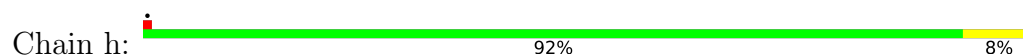
- Molecule 37: 60S ribosomal protein L33-A



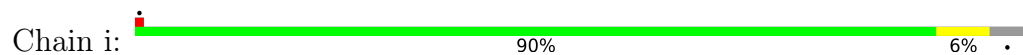
- Molecule 38: 60S ribosomal protein L34-A



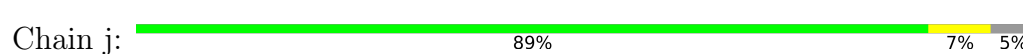
- Molecule 39: 60S ribosomal protein L35-A



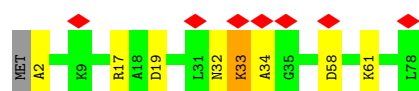
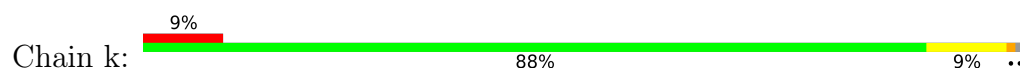
- Molecule 40: 60S ribosomal protein L36-A



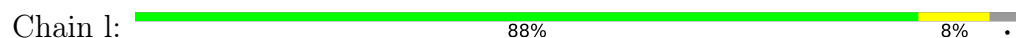
- Molecule 41: 60S ribosomal protein L37-A



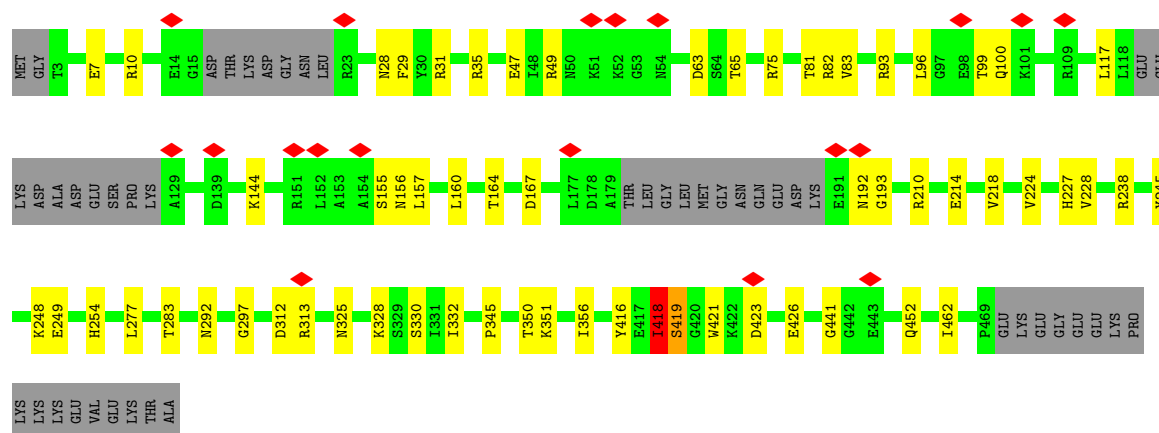
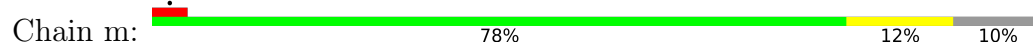
- Molecule 42: 60S ribosomal protein L38



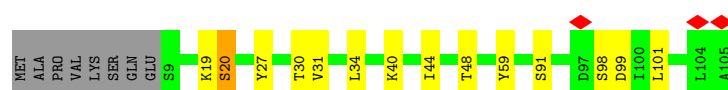
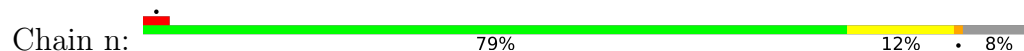
- Molecule 43: 60S ribosomal protein L39



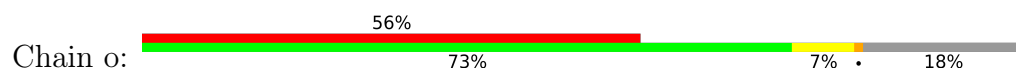
- Molecule 44: Nucleolar GTP-binding protein 2



- Molecule 45: 60S ribosomal protein L30



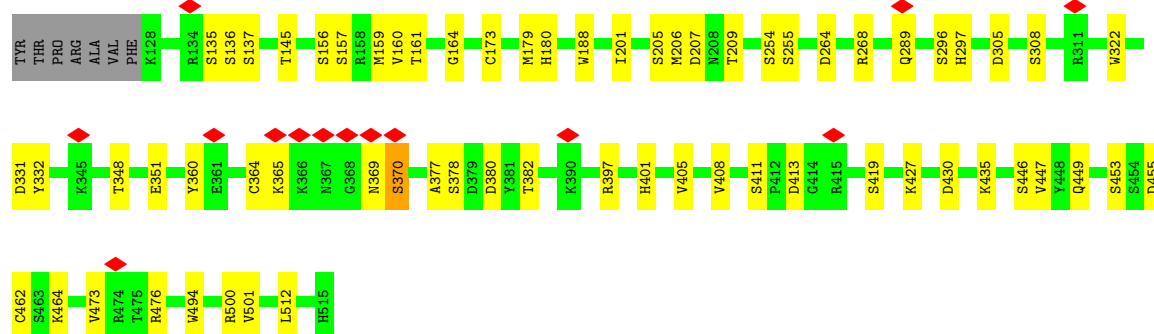
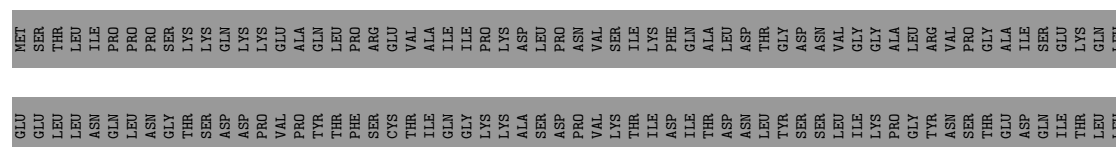
- Molecule 46: 60S ribosomal protein L1-A



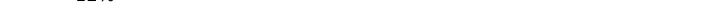


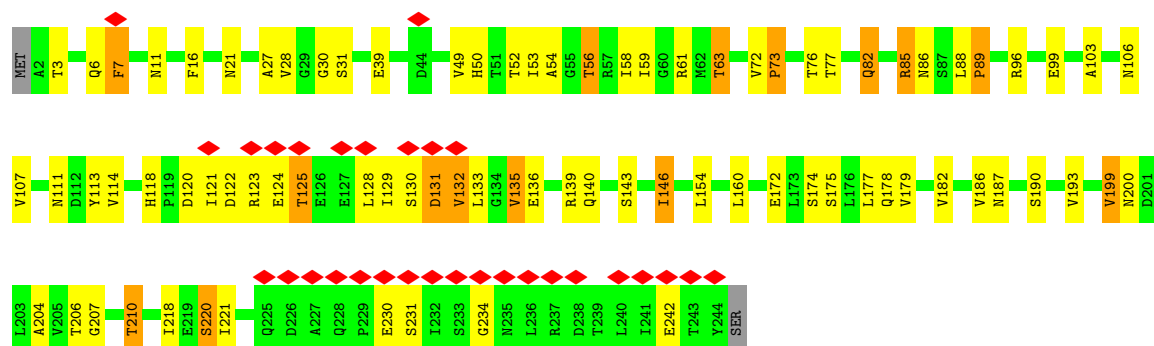
- Molecule 53: Ribosome assembly protein 4

Chain x: 63% 12% 25%

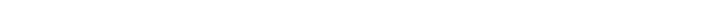


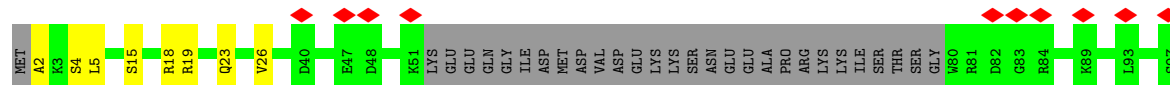
- Molecule 54: Eukaryotic translation initiation factor 6

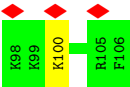
Chain γ : 



- Molecule 55: UPF0642 protein YBL028C

Chain z: 





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	114398	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	75	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.130	Depositor
Minimum map value	-0.049	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	423.6, 423.6, 423.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.059, 1.059, 1.059	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.18	1/72767 (0.0%)	0.36	27/113396 (0.0%)
2	2	0.17	0/3657	0.33	0/5692
3	3	0.13	0/2787	0.29	0/4339
4	4	0.21	0/4015	0.69	13/5447 (0.2%)
5	5	0.24	0/685	0.71	3/895 (0.3%)
6	A	0.26	0/1897	0.57	3/2550 (0.1%)
7	B	0.28	0/3152	0.71	5/4239 (0.1%)
8	C	0.24	0/2801	0.54	0/3792
9	D	0.21	0/2013	0.64	9/2715 (0.3%)
10	E	0.22	0/1260	0.59	5/1694 (0.3%)
11	F	0.23	0/1781	0.55	0/2396
12	G	0.25	0/1816	0.54	1/2450 (0.0%)
13	H	0.22	0/1507	0.53	0/2029
14	I	0.22	0/1067	0.67	2/1433 (0.1%)
15	J	0.23	0/1365	0.75	10/1831 (0.5%)
16	K	0.20	0/1903	0.69	9/2561 (0.4%)
17	L	0.26	0/1480	0.61	1/1986 (0.1%)
18	M	0.22	0/1055	0.53	2/1421 (0.1%)
19	N	0.26	0/1757	0.53	0/2354
20	O	0.24	0/1585	0.53	2/2128 (0.1%)
21	P	0.26	0/1382	0.49	0/1856
22	Q	0.24	0/1127	0.48	0/1521
23	R	0.25	0/1236	0.52	2/1650 (0.1%)
24	S	0.25	0/1473	0.61	2/1980 (0.1%)
25	T	0.23	0/997	0.71	3/1336 (0.2%)
26	U	0.22	0/817	0.54	0/1109
27	V	0.39	0/1008	1.50	25/1356 (1.8%)
28	W	0.21	0/1910	0.53	0/2575
29	X	0.22	0/1108	0.48	0/1492
30	Y	0.23	0/995	0.58	2/1329 (0.2%)
31	Z	0.25	0/1118	0.61	1/1497 (0.1%)
32	a	0.23	0/751	0.57	0/1013

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	b	0.23	0/5032	0.80	30/6756 (0.4%)
34	c	0.20	0/879	0.65	6/1171 (0.5%)
35	d	0.23	0/870	0.61	3/1168 (0.3%)
36	e	0.22	0/1041	0.43	0/1394
37	f	0.25	0/868	0.45	0/1168
38	g	0.25	0/856	0.56	0/1144
39	h	0.23	0/978	0.47	0/1301
40	i	0.23	0/749	0.61	2/995 (0.2%)
41	j	0.25	0/680	0.52	0/901
42	k	0.24	0/618	0.49	0/826
43	l	0.27	0/435	0.49	0/577
44	m	0.24	0/3617	0.67	5/4870 (0.1%)
45	n	0.19	0/751	0.59	3/1008 (0.3%)
46	o	0.20	0/872	0.97	13/1208 (1.1%)
47	p	0.23	0/687	0.51	0/915
48	q	0.23	0/969	0.59	0/1301
49	r	0.26	0/1850	0.60	0/2472
50	s	0.21	0/467	0.65	1/609 (0.2%)
51	t	0.19	0/3447	0.54	6/4643 (0.1%)
52	u	0.24	0/1269	0.83	5/1687 (0.3%)
53	x	0.21	0/3111	0.55	6/4218 (0.1%)
54	y	0.31	0/1864	1.35	41/2538 (1.6%)
55	z	0.19	0/650	0.56	0/854
All	All	0.21	1/156832 (0.0%)	0.52	248/227786 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	4	0	4
5	5	0	3
6	A	0	4
7	B	0	3
9	D	0	3
10	E	0	1
11	F	0	2
12	G	0	2
13	H	0	1
14	I	0	1
15	J	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
16	K	0	3
17	L	0	1
18	M	0	1
24	S	0	4
25	T	0	4
27	V	0	7
28	W	0	1
30	Y	0	1
31	Z	0	2
33	b	0	11
34	c	0	1
40	i	0	1
42	k	0	2
44	m	0	1
45	n	0	1
46	o	0	6
47	p	0	1
48	q	0	2
49	r	0	1
52	u	0	1
54	y	0	5
All	All	0	84

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2318	U	C1'-N1	6.74	1.57	1.47

All (248) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	b	385	LEU	CA-C-N	16.00	144.75	122.19
33	b	385	LEU	C-N-CA	16.00	144.75	122.19
27	V	23	MET	CA-C-N	12.56	138.55	120.71
27	V	23	MET	C-N-CA	12.56	138.55	120.71
52	u	23	ARG	CA-C-N	12.38	140.41	120.60
52	u	23	ARG	C-N-CA	12.38	140.41	120.60
54	y	54	ALA	CA-C-N	12.31	142.19	120.77
54	y	54	ALA	C-N-CA	12.31	142.19	120.77
27	V	36	ILE	CA-C-N	11.28	134.81	120.70
27	V	36	ILE	C-N-CA	11.28	134.81	120.70
54	y	77	THR	CA-C-N	10.99	135.44	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	y	77	THR	C-N-CA	10.99	135.44	120.38
4	4	544	ASN	O-C-N	-10.16	109.63	121.32
54	y	73	PRO	CA-C-N	9.71	133.29	120.28
54	y	73	PRO	C-N-CA	9.71	133.29	120.28
6	A	143	GLU	O-C-N	-9.62	111.03	122.58
44	m	193	GLY	CA-C-N	9.48	138.97	121.62
44	m	193	GLY	C-N-CA	9.48	138.97	121.62
54	y	146	ILE	CA-C-N	9.24	136.47	122.23
54	y	146	ILE	C-N-CA	9.24	136.47	122.23
7	B	58	ARG	CA-C-N	9.20	134.80	122.84
7	B	58	ARG	C-N-CA	9.20	134.80	122.84
33	b	229	THR	CA-C-N	-9.14	108.03	122.65
33	b	229	THR	C-N-CA	-9.14	108.03	122.65
33	b	163	ILE	O-C-N	-8.91	113.76	123.20
25	T	69	LYS	CA-C-N	-8.86	110.77	126.45
25	T	69	LYS	C-N-CA	-8.86	110.77	126.45
33	b	226	ASP	O-C-N	-8.70	110.92	122.23
33	b	576	SER	O-C-N	-8.63	111.11	122.59
45	n	20	SER	O-C-N	-8.61	109.64	122.81
4	4	43	THR	CA-C-N	8.59	131.98	120.65
4	4	43	THR	C-N-CA	8.59	131.98	120.65
53	x	369	ASN	CA-C-N	-8.57	109.89	122.65
53	x	369	ASN	C-N-CA	-8.57	109.89	122.65
7	B	348	ARG	CA-CB-CG	8.52	131.13	114.10
27	V	14	SER	CA-C-N	8.41	134.06	122.19
27	V	14	SER	C-N-CA	8.41	134.06	122.19
30	Y	6	LEU	CA-C-N	8.39	131.52	120.28
30	Y	6	LEU	C-N-CA	8.39	131.52	120.28
16	K	166	ASP	O-C-N	-8.38	112.33	122.48
46	o	87	VAL	CA-C-N	-8.35	109.29	122.65
46	o	87	VAL	C-N-CA	-8.35	109.29	122.65
25	T	54	HIS	O-C-N	-8.32	111.52	122.59
54	y	131	ASP	O-C-N	-8.32	113.62	122.19
52	u	128	GLU	CA-C-N	8.17	131.74	120.63
52	u	128	GLU	C-N-CA	8.17	131.74	120.63
54	y	99	GLU	CA-C-N	8.04	131.06	120.28
54	y	99	GLU	C-N-CA	8.04	131.06	120.28
15	J	143	ARG	CA-C-N	-7.95	110.68	124.82
15	J	143	ARG	C-N-CA	-7.95	110.68	124.82
46	o	14	LYS	CA-C-N	-7.83	108.20	122.38
46	o	14	LYS	C-N-CA	-7.83	108.20	122.38
33	b	341	ALA	CA-C-N	-7.82	108.22	122.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	b	341	ALA	C-N-CA	-7.82	108.22	122.38
16	K	165	GLY	CA-C-N	-7.80	109.31	122.11
16	K	165	GLY	C-N-CA	-7.80	109.31	122.11
4	4	491	SER	O-C-N	-7.75	112.28	122.59
1	1	2338	C	C2'-C3'-O3'	7.74	125.31	113.70
16	K	309	GLU	CA-C-N	7.70	132.64	120.47
16	K	309	GLU	C-N-CA	7.70	132.64	120.47
31	Z	27	LYS	O-C-N	7.66	130.13	121.32
51	t	24	ASP	O-C-N	-7.62	113.77	121.31
33	b	72	ASN	CA-C-N	-7.61	112.22	123.93
33	b	72	ASN	C-N-CA	-7.61	112.22	123.93
27	V	134	GLY	CA-C-N	7.59	133.30	123.13
27	V	134	GLY	C-N-CA	7.59	133.30	123.13
4	4	461	ASP	O-C-N	-7.58	114.00	122.34
33	b	430	ASP	CA-C-N	7.57	133.47	122.94
33	b	430	ASP	C-N-CA	7.57	133.47	122.94
17	L	165	SER	O-C-N	7.55	132.63	122.59
27	V	83	LYS	CA-C-N	7.49	134.80	122.07
27	V	83	LYS	C-N-CA	7.49	134.80	122.07
54	y	218	ILE	CA-C-N	7.47	130.29	120.28
54	y	218	ILE	C-N-CA	7.47	130.29	120.28
54	y	85	ARG	CA-C-N	7.42	130.83	120.29
54	y	85	ARG	C-N-CA	7.42	130.83	120.29
54	y	124	GLU	CA-C-N	-7.36	109.06	122.38
54	y	124	GLU	C-N-CA	-7.36	109.06	122.38
9	D	167	SER	CA-C-N	7.34	130.45	120.54
9	D	167	SER	C-N-CA	7.34	130.45	120.54
54	y	82	GLN	CA-C-N	7.28	129.91	120.44
54	y	82	GLN	C-N-CA	7.28	129.91	120.44
50	s	12	SER	O-C-N	7.26	132.24	122.59
33	b	162	SER	CA-C-N	7.23	132.71	123.10
33	b	162	SER	C-N-CA	7.23	132.71	123.10
33	b	540	HIS	CA-C-N	-7.17	111.55	122.81
33	b	540	HIS	C-N-CA	-7.17	111.55	122.81
53	x	135	SER	CA-C-N	7.12	135.47	122.02
53	x	135	SER	C-N-CA	7.12	135.47	122.02
35	d	47	ASP	CA-C-N	-7.09	112.20	122.19
35	d	47	ASP	C-N-CA	-7.09	112.20	122.19
27	V	37	ILE	N-CA-C	7.07	117.16	110.30
27	V	12	ARG	CA-C-N	7.06	132.75	122.94
27	V	12	ARG	C-N-CA	7.06	132.75	122.94
40	i	63	ASN	CA-C-N	7.04	134.09	121.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	i	63	ASN	C-N-CA	7.04	134.09	121.92
24	S	84	ARG	CA-C-N	7.02	134.95	121.54
24	S	84	ARG	C-N-CA	7.02	134.95	121.54
54	y	61	ARG	CA-C-N	7.02	134.02	121.66
54	y	61	ARG	C-N-CA	7.02	134.02	121.66
10	E	141	VAL	CA-C-N	-6.98	109.07	122.06
10	E	141	VAL	C-N-CA	-6.98	109.07	122.06
1	1	3048	A	O4'-C1'-N9	6.90	118.55	108.20
5	5	66	ASP	O-C-N	-6.85	113.16	122.33
27	V	111	GLY	CA-C-N	-6.85	111.49	122.24
27	V	111	GLY	C-N-CA	-6.85	111.49	122.24
10	E	14	ASP	CA-C-N	-6.84	114.32	122.93
10	E	14	ASP	C-N-CA	-6.84	114.32	122.93
1	1	2339	C	N1-C1'-C2'	6.77	124.16	114.00
1	1	2338	C	C1'-C2'-O2'	6.75	118.53	108.40
9	D	234	ASP	CA-C-N	6.67	130.06	120.79
9	D	234	ASP	C-N-CA	6.67	130.06	120.79
46	o	85	MET	CA-C-N	6.66	132.81	120.95
46	o	85	MET	C-N-CA	6.66	132.81	120.95
27	V	13	ILE	O-C-N	-6.65	115.98	123.10
54	y	130	SER	CA-C-N	-6.64	111.82	121.98
54	y	130	SER	C-N-CA	-6.64	111.82	121.98
16	K	296	PHE	CA-C-N	6.62	129.14	120.60
16	K	296	PHE	C-N-CA	6.62	129.14	120.60
1	1	1897	G	N9-C1'-C2'	6.61	121.92	112.00
27	V	36	ILE	CA-CB-CG1	6.61	121.64	110.40
18	M	97	SER	CA-C-N	6.60	130.72	120.82
18	M	97	SER	C-N-CA	6.60	130.72	120.82
33	b	181	SER	CA-C-N	-6.52	108.86	121.58
33	b	181	SER	C-N-CA	-6.52	108.86	121.58
46	o	40	ASN	O-C-N	-6.51	113.93	122.59
54	y	121	ILE	N-CA-C	6.46	118.75	109.51
44	m	418	ILE	O-C-N	6.46	130.64	122.57
33	b	546	GLN	CA-C-N	6.44	129.23	120.54
33	b	546	GLN	C-N-CA	6.44	129.23	120.54
33	b	225	LEU	CA-C-N	-6.42	109.61	120.58
33	b	225	LEU	C-N-CA	-6.42	109.61	120.58
27	V	90	GLY	N-CA-C	6.34	117.50	111.67
54	y	220	SER	CA-C-N	6.33	131.14	120.64
54	y	220	SER	C-N-CA	6.33	131.14	120.64
15	J	144	CYS	O-C-N	-6.27	114.07	121.97
9	D	231	ILE	CA-C-N	6.23	133.45	122.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	231	ILE	C-N-CA	6.23	133.45	122.67
33	b	398	LEU	O-C-N	6.22	130.86	122.59
4	4	460	TYR	CA-C-N	-6.20	112.50	122.24
4	4	460	TYR	C-N-CA	-6.20	112.50	122.24
1	1	1896	A	N9-C1'-C2'	6.18	121.27	112.00
12	G	200	LEU	O-C-N	6.16	130.44	123.42
1	1	2339	C	C5'-C4'-C3'	6.11	124.36	115.20
54	y	200	ASN	N-CA-C	6.09	116.13	108.45
1	1	1896	A	C3'-C2'-O2'	6.08	119.82	110.70
27	V	85	TRP	CA-CB-CG	6.07	125.13	113.60
14	I	11	THR	CA-CB-CG2	6.05	120.78	110.50
54	y	199	VAL	N-CA-C	6.04	117.05	108.42
1	1	1896	A	C1'-C2'-O2'	6.04	117.45	108.40
1	1	2339	C	C4'-C3'-O3'	6.03	118.45	109.40
4	4	463	THR	CA-C-N	-5.99	114.25	122.93
4	4	463	THR	C-N-CA	-5.99	114.25	122.93
46	o	103	LEU	CA-C-N	5.94	129.74	120.82
46	o	103	LEU	C-N-CA	5.94	129.74	120.82
1	1	1901	A	C3'-C2'-O2'	5.93	119.59	110.70
27	V	18	PRO	N-CA-C	5.89	119.76	111.33
1	1	3039	C	N1-C1'-C2'	5.88	120.82	112.00
1	1	1900	A	C1'-C2'-O2'	5.85	120.58	111.80
54	y	56	THR	OG1-CB-CG2	5.82	120.93	109.30
53	x	370	SER	O-C-N	5.81	129.99	123.19
4	4	490	ASN	CA-C-N	5.81	132.63	121.54
4	4	490	ASN	C-N-CA	5.81	132.63	121.54
20	O	136	THR	CA-C-N	-5.81	113.69	122.81
20	O	136	THR	C-N-CA	-5.81	113.69	122.81
34	c	84	ILE	CA-C-N	5.80	131.69	122.59
34	c	84	ILE	C-N-CA	5.80	131.69	122.59
27	V	112	SER	O-C-N	-5.79	115.97	122.34
33	b	329	MET	CA-C-N	5.79	128.83	120.79
33	b	329	MET	C-N-CA	5.79	128.83	120.79
1	1	3039	C	C5'-C4'-C3'	5.78	124.67	116.00
7	B	386	ASP	O-C-N	5.77	130.26	122.59
1	1	1901	A	C1'-C2'-O2'	5.76	117.04	108.40
51	t	23	ARG	CA-C-N	5.72	130.02	123.21
51	t	23	ARG	C-N-CA	5.72	130.02	123.21
1	1	1900	A	C3'-C2'-O2'	5.68	123.12	114.60
1	1	1897	G	C5'-C4'-C3'	5.67	124.50	116.00
15	J	22	SER	O-C-N	-5.66	116.14	122.93
51	t	161	SER	CA-C-N	5.65	128.90	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	t	161	SER	C-N-CA	5.65	128.90	120.31
1	1	2338	C	C4'-C3'-O3'	5.64	121.47	113.00
9	D	66	SER	CA-C-N	-5.64	113.59	122.73
9	D	66	SER	C-N-CA	-5.64	113.59	122.73
4	4	94	THR	OG1-CB-CG2	5.62	120.55	109.30
1	1	1898	G	C5'-C4'-C3'	5.62	124.42	116.00
27	V	61	THR	OG1-CB-CG2	5.62	120.53	109.30
54	y	63	THR	OG1-CB-CG2	5.59	120.48	109.30
34	c	21	HIS	CA-C-N	5.56	128.52	120.79
34	c	21	HIS	C-N-CA	5.56	128.52	120.79
54	y	210	THR	OG1-CB-CG2	5.54	120.38	109.30
53	x	322	TRP	CA-CB-CG	5.54	124.12	113.60
27	V	101	VAL	CG1-CB-CG2	5.52	122.94	110.80
54	y	3	THR	OG1-CB-CG2	5.50	120.30	109.30
5	5	65	LYS	CA-C-N	-5.48	111.36	120.68
5	5	65	LYS	C-N-CA	-5.48	111.36	120.68
54	y	230	GLU	CA-C-N	-5.48	113.96	122.67
54	y	230	GLU	C-N-CA	-5.48	113.96	122.67
54	y	136	GLU	N-CA-C	5.47	118.01	110.35
45	n	19	LYS	CA-C-N	5.46	131.65	123.24
45	n	19	LYS	C-N-CA	5.46	131.65	123.24
54	y	30	GLY	CA-C-N	5.44	131.35	122.81
54	y	30	GLY	C-N-CA	5.44	131.35	122.81
16	K	35	SER	O-C-N	5.43	129.90	123.33
1	1	2338	C	C3'-C2'-O2'	5.43	118.84	110.70
23	R	129	GLY	CA-C-N	-5.40	111.22	121.54
23	R	129	GLY	C-N-CA	-5.40	111.22	121.54
35	d	48	ASP	O-C-N	5.40	129.37	123.22
14	I	11	THR	OG1-CB-CG2	5.38	120.06	109.30
9	D	67	SER	O-C-N	5.37	129.82	123.27
1	1	3042	U	C5'-C4'-O4'	5.37	117.85	109.80
4	4	44	SER	O-C-N	5.37	127.61	122.03
10	E	142	ASP	O-C-N	-5.37	114.78	122.41
1	1	2335	G	O4'-C1'-N9	5.35	116.22	108.20
7	B	103	THR	O-C-N	5.33	129.44	123.48
1	1	1898	G	C5'-C4'-O4'	5.32	117.79	109.80
46	o	19	TYR	CA-C-N	5.31	131.69	121.54
46	o	19	TYR	C-N-CA	5.31	131.69	121.54
33	b	575	ALA	CA-C-N	5.30	131.66	121.54
33	b	575	ALA	C-N-CA	5.30	131.66	121.54
1	1	3042	U	C5'-C4'-C3'	5.28	123.92	116.00
15	J	21	ILE	CA-C-N	5.26	129.41	122.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	J	21	ILE	C-N-CA	5.26	129.41	122.42
54	y	125	THR	O-C-N	-5.24	115.14	122.37
27	V	61	THR	CA-CB-CG2	5.23	119.39	110.50
44	m	29	PHE	CA-C-N	5.21	132.60	121.45
44	m	29	PHE	C-N-CA	5.21	132.60	121.45
34	c	111	VAL	CA-C-N	5.20	129.46	121.19
34	c	111	VAL	C-N-CA	5.20	129.46	121.19
51	t	338	ASP	O-C-N	5.20	127.30	121.32
54	y	49	VAL	CG1-CB-CG2	5.18	122.20	110.80
54	y	89	PRO	N-CA-C	5.17	118.72	111.33
33	b	73	ASP	O-C-N	-5.16	114.17	121.91
15	J	118	PRO	CA-C-N	5.15	131.38	121.54
15	J	118	PRO	C-N-CA	5.15	131.38	121.54
15	J	169	ALA	CA-C-N	5.15	132.25	123.03
15	J	169	ALA	C-N-CA	5.15	132.25	123.03
54	y	58	ILE	CG1-CB-CG2	5.14	126.12	110.70
52	u	77	VAL	CG1-CB-CG2	5.14	122.10	110.80
16	K	86	LYS	O-C-N	-5.12	116.16	122.82
1	1	1899	G	C5'-C4'-C3'	5.11	122.86	115.20
33	b	342	SER	O-C-N	-5.09	115.34	122.37
46	o	191	VAL	CA-C-N	5.09	127.41	120.54
46	o	191	VAL	C-N-CA	5.09	127.41	120.54
1	1	2335	G	N9-C1'-C2'	5.06	121.59	114.00
27	V	77	ILE	CG1-CB-CG2	5.06	125.87	110.70
6	A	142	ASP	CA-C-N	-5.03	115.35	122.34
6	A	142	ASP	C-N-CA	-5.03	115.35	122.34
1	1	3094	A	C4'-C3'-O3'	5.00	120.50	113.00

There are no chirality outliers.

All (84) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	4	329	CYS	Mainchain
4	4	362	ARG	Peptide
4	4	461	ASP	Mainchain
4	4	463	THR	Peptide
5	5	116	ALA	Peptide
5	5	42	THR	Mainchain
5	5	66	ASP	Mainchain
6	A	143	GLU	Mainchain,Peptide
6	A	221	LYS	Peptide
6	A	230	VAL	Peptide

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Mol	Chain	Res	Type	Group
7	B	155	ALA	Peptide
7	B	221	THR	Peptide
7	B	340	LYS	Peptide
9	D	168	ASP	Mainchain
9	D	235	SER	Mainchain
9	D	242	SER	Mainchain
10	E	142	ASP	Mainchain
11	F	158	LYS	Peptide
11	F	190	THR	Peptide
12	G	158	ASP	Mainchain
12	G	76	ALA	Peptide
13	H	21	LYS	Peptide
14	I	15	THR	Peptide
15	J	119	SER	Mainchain
15	J	144	CYS	Mainchain
15	J	34	SER	Mainchain
16	K	166	ASP	Mainchain
16	K	297	ILE	Mainchain
16	K	310	VAL	Mainchain
17	L	46	ILE	Peptide
18	M	98	SER	Mainchain
24	S	12	ARG	Peptide
24	S	155	ARG	Peptide
24	S	18	SER	Mainchain
24	S	22	PRO	Peptide
25	T	53	PRO	Peptide
25	T	54	HIS	Mainchain
25	T	70	SER	Mainchain,Peptide
27	V	100	GLY	Peptide
27	V	101	VAL	Peptide
27	V	35	TYR	Peptide
27	V	37	ILE	Mainchain,Peptide
27	V	76	ALA	Peptide
27	V	99	ALA	Peptide
28	W	176	LYS	Peptide
30	Y	7	ASP	Mainchain
31	Z	101	PHE	Peptide
31	Z	102	GLU	Peptide
33	b	182	SER	Mainchain
33	b	2	GLN	Peptide
33	b	226	ASP	Mainchain,Peptide
33	b	230	GLU	Mainchain

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Mol	Chain	Res	Type	Group
33	b	248	SER	Peptide
33	b	321	SER	Peptide
33	b	342	SER	Mainchain
33	b	367	GLN	Peptide
33	b	547	ASP	Mainchain
33	b	73	ASP	Mainchain
34	c	112	ASP	Mainchain
40	i	64	SER	Mainchain
42	k	33	LYS	Peptide
42	k	34	ALA	Peptide
44	m	418	ILE	Peptide
45	n	20	SER	Mainchain
46	o	104	SER	Mainchain
46	o	15	GLU	Mainchain
46	o	20	SER	Mainchain
46	o	40	ASN	Mainchain
46	o	80	CYS	Mainchain
46	o	88	ASP	Mainchain
47	p	60	CYS	Mainchain
48	q	143	VAL	Peptide
48	q	16	ARG	Peptide
49	r	145	LYS	Peptide
52	u	129	SER	Mainchain
54	y	125	THR	Mainchain
54	y	131	ASP	Mainchain
54	y	132	VAL	Mainchain
54	y	50	HIS	Peptide
54	y	7	PHE	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	65028	0	32701	287	0
2	2	3273	0	1654	7	0
3	3	2494	0	1262	19	0
4	4	3945	0	4016	99	0
5	5	681	0	732	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	1863	0	1930	18	0
7	B	3081	0	3165	29	0
8	C	2749	0	2863	24	0
9	D	1969	0	1926	62	0
10	E	1239	0	1326	11	0
11	F	1744	0	1824	25	0
12	G	1784	0	1883	22	0
13	H	1486	0	1559	15	0
14	I	1051	0	1077	14	0
15	J	1344	0	1370	33	0
16	K	1875	0	1979	26	0
17	L	1456	0	1517	23	0
18	M	1040	0	1131	18	0
19	N	1720	0	1779	21	0
20	O	1555	0	1659	4	0
21	P	1360	0	1394	27	0
22	Q	1110	0	1190	19	0
23	R	1219	0	1300	22	0
24	S	1437	0	1475	22	0
25	T	983	0	1037	41	0
26	U	800	0	811	5	0
27	V	993	0	1040	54	0
28	W	1877	0	1910	11	0
29	X	1092	0	1176	8	0
30	Y	984	0	1075	9	0
31	Z	1092	0	1155	17	0
32	a	735	0	776	10	0
33	b	4953	0	4993	108	0
34	c	872	0	940	25	0
35	d	856	0	904	7	0
36	e	1020	0	1090	7	0
37	f	850	0	880	7	0
38	g	846	0	910	14	0
39	h	969	0	1078	6	0
40	i	743	0	822	3	0
41	j	665	0	668	5	0
42	k	612	0	682	20	0
43	l	428	0	464	3	0
44	m	3546	0	3627	54	0
45	n	743	0	797	8	0
46	o	877	0	377	6	0
47	p	680	0	724	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	q	961	0	1010	15	0
49	r	1818	0	1925	18	0
50	s	463	0	522	3	0
51	t	3395	0	3497	41	0
52	u	1247	0	1299	13	0
53	x	3033	0	2980	43	0
54	y	1841	0	1824	57	0
55	z	643	0	693	9	0
56	I	1	0	0	0	0
56	j	1	0	0	0	0
56	p	1	0	0	0	0
56	u	1	0	0	0	0
57	b	32	0	12	2	0
57	m	32	0	12	3	0
58	b	1	0	0	0	0
58	m	1	0	0	0	0
All	All	147190	0	114422	1252	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 5.

All (1252) 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)
23:R:95:TRP:HZ3	23:R:98:ARG:NH2	1.23	1.29
23:R:95:TRP:CZ3	23:R:98:ARG:NH2	2.03	1.26
53:x:364:CYS:SG	53:x:370:SER:OG	1.94	1.24
34:c:109:LEU:HA	34:c:112:ASP:OD2	1.42	1.17
1:1:2722:U:OP1	25:T:88:ARG:NH1	1.79	1.16
21:P:8:SER:OG	34:c:85:THR:OG1	1.65	1.15
9:D:67:SER:HB3	9:D:72:ASP:OD1	1.53	1.08
33:b:420:TYR:OH	33:b:428:LYS:HA	1.54	1.08
42:k:32:ASN:CG	42:k:33:LYS:NZ	2.10	1.08
9:D:67:SER:CA	9:D:72:ASP:OD1	2.00	1.08
6:A:142:ASP:O	6:A:143:GLU:HG3	1.53	1.07
9:D:67:SER:HA	9:D:72:ASP:OD1	1.54	1.06
25:T:69:LYS:O	25:T:70:SER:OG	1.74	1.06
27:V:36:ILE:HG13	27:V:60:ALA:HA	1.37	1.05
25:T:54:HIS:NE2	25:T:89:LEU:CD2	2.19	1.05
44:m:96:LEU:HA	44:m:99:THR:HG22	1.37	1.05
27:V:36:ILE:HG13	27:V:60:ALA:CA	1.87	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:466:LEU:O	4:4:467:THR:OG1	1.76	1.03
16:K:294:ALA:O	16:K:297:ILE:HG22	1.58	1.02
9:D:67:SER:CB	9:D:72:ASP:OD1	2.07	1.01
5:5:42:THR:OG1	5:5:45:GLU:HB3	1.62	1.00
15:J:90:GLN:HG2	15:J:170:ASP:OD2	1.61	0.99
44:m:96:LEU:HD23	44:m:99:THR:HG21	1.45	0.98
12:G:78:PHE:O	12:G:79:GLN:HG2	1.64	0.98
33:b:398:LEU:CD2	54:y:39:GLU:HB3	1.94	0.98
54:y:132:VAL:HG13	54:y:133:LEU:HD12	1.40	0.97
25:T:54:HIS:NE2	25:T:89:LEU:HD21	1.79	0.97
33:b:420:TYR:OH	33:b:428:LYS:CA	2.13	0.97
42:k:32:ASN:CG	42:k:33:LYS:HZ1	1.72	0.96
24:S:17:GLU:O	24:S:18:SER:OG	1.81	0.95
52:u:126:LEU:O	52:u:129:SER:OG	1.84	0.95
54:y:129:ILE:HA	54:y:132:VAL:HG12	1.48	0.94
42:k:32:ASN:O	42:k:33:LYS:NZ	1.98	0.94
7:B:57:VAL:HG22	7:B:73:VAL:HG22	1.47	0.94
33:b:420:TYR:HE2	33:b:428:LYS:CE	1.80	0.94
42:k:32:ASN:CB	42:k:33:LYS:NZ	2.29	0.94
1:1:69:C:HO2'	1:1:101:G:HO2'	1.13	0.94
33:b:398:LEU:HD22	54:y:39:GLU:HB3	1.48	0.93
12:G:158:ASP:CG	12:G:159:PRO:HD3	1.93	0.93
18:M:65:LEU:HD12	24:S:172:TYR:HE2	1.34	0.92
1:1:2856:G:H21	49:r:192:THR:HG21	1.33	0.92
16:K:307:LYS:O	16:K:310:VAL:HG22	1.70	0.92
9:D:67:SER:HB3	9:D:72:ASP:CG	1.95	0.90
5:5:43:SER:O	5:5:46:LEU:CD2	2.20	0.89
25:T:54:HIS:HB3	25:T:57:TYR:HB2	1.54	0.89
34:c:109:LEU:HA	34:c:112:ASP:CG	1.95	0.89
42:k:32:ASN:O	42:k:33:LYS:CE	2.21	0.89
44:m:245:TYR:CE1	44:m:249:GLU:HG2	2.08	0.89
1:1:2891:U:HO2'	55:z:2:ALA:N	1.69	0.89
27:V:85:TRP:CD2	27:V:93:LEU:HD11	2.06	0.89
15:J:31:THR:O	15:J:34:SER:HB3	1.74	0.88
9:D:99:TYR:OH	9:D:168:ASP:OD1	1.91	0.88
21:P:8:SER:CB	34:c:85:THR:OG1	2.22	0.87
15:J:119:SER:OG	15:J:120:ILE:HG23	1.72	0.87
34:c:109:LEU:O	34:c:112:ASP:HB2	1.74	0.87
42:k:32:ASN:HB2	42:k:33:LYS:HZ3	1.40	0.87
27:V:87:ARG:HG3	27:V:93:LEU:HD23	1.55	0.86
25:T:54:HIS:CE1	25:T:89:LEU:HD21	2.12	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:p:42:CYS:SG	47:p:60:CYS:HB2	2.16	0.85
9:D:99:TYR:CE1	9:D:168:ASP:OD1	2.30	0.84
53:x:136:SER:OG	53:x:137:SER:O	1.95	0.84
4:4:527:GLY:O	4:4:531:THR:HG21	1.78	0.84
19:N:110:ALA:HB1	19:N:113:LEU:HD23	1.59	0.84
9:D:232:ASP:C	9:D:235:SER:OG	2.21	0.84
12:G:158:ASP:CB	12:G:159:PRO:HD3	2.08	0.83
52:u:140:GLU:OE1	52:u:141:ILE:HG13	1.79	0.82
25:T:54:HIS:NE2	25:T:89:LEU:HD22	1.92	0.82
27:V:13:ILE:CD1	27:V:54:LEU:HD12	2.09	0.82
42:k:32:ASN:O	42:k:33:LYS:HE2	1.78	0.82
9:D:99:TYR:CZ	9:D:168:ASP:OD1	2.33	0.82
27:V:85:TRP:CD1	27:V:93:LEU:HD12	2.15	0.81
4:4:98:ASP:OD2	4:4:137:ASP:OD1	1.98	0.81
24:S:17:GLU:O	24:S:18:SER:CB	2.25	0.81
9:D:232:ASP:O	9:D:235:SER:OG	1.98	0.81
9:D:239:ILE:O	9:D:242:SER:HB3	1.80	0.81
27:V:13:ILE:HG13	27:V:54:LEU:HD13	1.62	0.81
4:4:475:LEU:HD11	4:4:480:VAL:CG2	2.10	0.81
42:k:32:ASN:CG	42:k:33:LYS:HZ2	1.88	0.81
17:L:131:LYS:HE2	17:L:131:LYS:H	1.46	0.80
4:4:328:HIS:O	4:4:329:CYS:SG	2.39	0.80
5:5:43:SER:O	5:5:46:LEU:HD21	1.80	0.80
42:k:32:ASN:HB2	42:k:33:LYS:NZ	1.96	0.79
46:o:17:LEU:O	46:o:20:SER:CB	2.30	0.79
9:D:103:LEU:HD23	9:D:247:ILE:HD11	1.64	0.79
12:G:158:ASP:HB3	12:G:159:PRO:CD	2.12	0.79
14:I:87:GLN:OE1	14:I:90:SER:OG	1.99	0.79
17:L:47:ALA:O	17:L:137:GLN:NE2	2.15	0.79
1:1:1671:C:OP1	23:R:60:LYS:NZ	2.16	0.78
9:D:232:ASP:HB2	9:D:235:SER:HB3	1.65	0.78
18:M:65:LEU:HD12	24:S:172:TYR:CE2	2.19	0.78
1:1:2267:C:O2'	1:1:2268:U:O2	2.02	0.78
4:4:328:HIS:O	4:4:329:CYS:CB	2.31	0.78
44:m:96:LEU:HA	44:m:99:THR:CG2	2.12	0.77
1:1:687:U:OP2	17:L:36:ARG:NH2	2.17	0.77
5:5:43:SER:O	5:5:46:LEU:HD23	1.85	0.77
1:1:1364:C:OP1	11:F:110:ARG:NH1	2.18	0.77
33:b:420:TYR:HE2	33:b:428:LYS:HE2	1.49	0.77
53:x:378:SER:OG	53:x:380:ASP:OD1	2.03	0.76
4:4:467:THR:HG21	33:b:575:ALA:H	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:D:232:ASP:C	9:D:235:SER:HG	1.94	0.75
12:G:158:ASP:CB	12:G:159:PRO:CD	2.63	0.75
46:o:79:SER:O	46:o:80:CYS:CB	2.31	0.75
1:1:76:G:O2'	17:L:100:ARG:NH1	2.19	0.75
1:1:1120:A:OP1	50:s:21:LYS:NZ	2.19	0.75
21:P:108:ASP:O	21:P:112:LEU:HD13	1.86	0.75
1:1:1412:G:OP1	36:e:105:ARG:NH2	2.19	0.75
2:2:95:G:OP2	41:j:72:ARG:NH1	2.20	0.75
33:b:305:LEU:HA	33:b:308:SER:OG	1.87	0.75
44:m:210:ARG:NH2	44:m:351:LYS:O	2.20	0.75
1:1:2929:C:O2'	1:1:2930:A:O5'	2.02	0.74
27:V:13:ILE:CD1	27:V:54:LEU:CD1	2.65	0.74
1:1:1639:C:OP2	38:g:74:ARG:NH2	2.20	0.74
23:R:105:LEU:HD23	23:R:138:LEU:HD23	1.68	0.74
44:m:245:TYR:HE1	44:m:249:GLU:HG2	1.52	0.74
3:3:7:G:O2'	9:D:71:GLY:O	2.04	0.74
1:1:2627:C:H42	1:1:2651:G:H22	1.34	0.74
27:V:36:ILE:HG13	27:V:60:ALA:C	2.13	0.74
44:m:96:LEU:CA	44:m:99:THR:HG22	2.15	0.74
19:N:192:LYS:O	19:N:196:THR:OG1	2.04	0.74
33:b:102:LYS:O	33:b:104:LEU:N	2.21	0.74
44:m:418:ILE:HD11	44:m:421:TRP:CZ3	2.23	0.74
54:y:132:VAL:CG1	54:y:133:LEU:N	2.51	0.74
1:1:292:U:OP2	19:N:68:ARG:NH2	2.21	0.74
1:1:3167:A:O2'	1:1:3168:A:O4'	2.05	0.74
33:b:324:LEU:HD11	33:b:327:ASN:HB3	1.69	0.74
1:1:3163:A:N6	1:1:3288:G:O4'	2.21	0.73
54:y:76:THR:O	54:y:96:ARG:NH2	2.20	0.73
1:1:1364:C:O2'	22:Q:9:GLN:OE1	2.05	0.73
1:1:2183:A:O2'	6:A:235:ALA:O	2.02	0.73
1:1:3070:A:OP1	23:R:62:ARG:NH2	2.20	0.73
1:1:3288:G:O2'	1:1:3290:G:N7	2.21	0.73
48:q:85:LEU:HG	48:q:104:ILE:HD11	1.70	0.73
54:y:85:ARG:NH2	54:y:89:PRO:O	2.22	0.73
1:1:117:U:O2'	1:1:119:U:OP2	2.06	0.73
9:D:232:ASP:HB2	9:D:235:SER:CB	2.19	0.73
25:T:54:HIS:HD2	25:T:57:TYR:CD2	2.06	0.73
1:1:210:U:O2'	1:1:229:G:O2'	2.07	0.73
1:1:990:U:O2'	1:1:991:G:OP1	2.05	0.73
48:q:76:SER:HG	48:q:79:SER:HG	1.32	0.73
46:o:39:LYS:O	46:o:40:ASN:CB	2.36	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:221:GLN:NE2	4:4:307:ASP:OD1	2.22	0.73
4:4:466:LEU:O	4:4:467:THR:CB	2.34	0.72
23:R:105:LEU:HD22	23:R:135:LYS:HD2	1.71	0.72
1:1:31:C:OP2	19:N:188:ARG:NH2	2.22	0.72
1:1:3212:C:OP2	18:M:124:ARG:NH2	2.22	0.72
1:1:1447:G:OP1	21:P:65:SER:OG	2.06	0.72
1:1:838:G:O6	47:p:4:ARG:NH2	2.22	0.72
4:4:527:GLY:O	4:4:531:THR:CG2	2.36	0.72
9:D:232:ASP:CA	9:D:235:SER:OG	2.38	0.72
33:b:180:LYS:NZ	33:b:221:THR:O	2.23	0.72
33:b:420:TYR:CE2	33:b:428:LYS:HD3	2.25	0.72
15:J:51:ARG:O	15:J:61:ARG:NH2	2.22	0.72
1:1:176:G:O6	1:1:242:C:N4	2.23	0.72
44:m:93:ARG:NH1	44:m:117:LEU:O	2.23	0.72
9:D:232:ASP:N	9:D:235:SER:OG	2.23	0.72
25:T:54:HIS:CE1	25:T:89:LEU:HD11	2.25	0.72
31:Z:53:VAL:HG21	31:Z:62:VAL:HG23	1.72	0.72
27:V:15:LEU:HD22	27:V:52:ALA:HA	1.71	0.72
27:V:87:ARG:CG	27:V:93:LEU:HD23	2.20	0.72
53:x:205:SER:OG	53:x:207:ASP:OD1	2.07	0.72
1:1:1316:C:OP2	20:O:133:ARG:NH1	2.23	0.71
1:1:3100:U:OP1	55:z:18:ARG:NH2	2.22	0.71
9:D:240:TYR:O	9:D:244:HIS:ND1	2.23	0.71
1:1:103:G:OP1	17:L:70:ARG:NH2	2.22	0.71
1:1:289:A:O2'	19:N:93:LYS:O	2.07	0.71
4:4:475:LEU:HD11	4:4:480:VAL:HG21	1.71	0.71
47:p:59:CYS:O	47:p:60:CYS:CB	2.37	0.71
3:3:119:U:OP1	9:D:256:THR:OG1	2.06	0.71
54:y:132:VAL:HG13	54:y:133:LEU:N	2.05	0.71
54:y:140:GLN:NE2	54:y:172:GLU:OE2	2.24	0.71
16:K:63:LYS:NZ	16:K:96:GLN:OE1	2.19	0.71
33:b:440:ASN:N	33:b:440:ASN:OD1	2.24	0.71
33:b:420:TYR:HE2	33:b:428:LYS:CD	2.04	0.71
1:1:520:U:OP2	11:F:70:LYS:NZ	2.24	0.71
4:4:466:LEU:C	4:4:467:THR:HG23	2.16	0.71
1:1:1631:C:OP2	31:Z:48:ARG:NH2	2.24	0.70
23:R:105:LEU:HD22	23:R:135:LYS:CD	2.20	0.70
1:1:1348:U:OP1	22:Q:39:ARG:NH1	2.24	0.70
27:V:33:ASN:O	27:V:34:LEU:HD23	1.92	0.70
1:1:438:A:OP1	36:e:118:LYS:NZ	2.24	0.70
53:x:156:SER:O	53:x:500:ARG:NH1	2.23	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1147:G:OP1	36:e:47:ARG:NH1	2.23	0.70
11:F:74:SER:OG	25:T:141:VAL:O	2.09	0.70
11:F:156:ILE:HD11	11:F:168:ILE:HG23	1.73	0.70
1:1:1657:C:O2'	1:1:1797:A:OP2	2.09	0.70
15:J:117:ASP:OD1	15:J:119:SER:OG	2.08	0.70
25:T:69:LYS:O	25:T:70:SER:CB	2.35	0.70
33:b:72:ASN:O	33:b:73:ASP:CB	2.39	0.70
1:1:424:G:O2'	36:e:23:ASP:OD2	2.10	0.70
26:U:91:ASP:O	33:b:526:LYS:NZ	2.25	0.70
1:1:1329:U:O2'	1:1:1330:A:OP1	2.08	0.69
1:1:2538:U:O2'	1:1:2541:U:O4	2.10	0.69
16:K:70:ARG:NH1	16:K:103:ASP:OD1	2.25	0.69
49:r:3:GLN:O	49:r:4:ASN:ND2	2.24	0.69
54:y:63:THR:HG22	54:y:72:VAL:HG12	1.73	0.69
54:y:82:GLN:OE1	54:y:86:ASN:ND2	2.24	0.69
17:L:131:LYS:H	17:L:131:LYS:CE	2.04	0.69
27:V:36:ILE:CD1	27:V:73:VAL:HG22	2.22	0.69
28:W:186:TYR:OH	28:W:198:ARG:NH1	2.25	0.69
44:m:7:GLU:OE1	44:m:10:ARG:NH2	2.25	0.69
33:b:324:LEU:O	33:b:324:LEU:HD12	1.92	0.69
4:4:141:ILE:O	4:4:155:SER:HB2	1.92	0.69
23:R:95:TRP:CZ3	23:R:98:ARG:CZ	2.73	0.69
19:N:31:ARG:NH1	19:N:124:ASP:OD2	2.25	0.69
48:q:81:VAL:O	48:q:85:LEU:HD12	1.92	0.69
1:1:389:A:OP1	21:P:4:TYR:OH	2.07	0.69
7:B:10:ARG:NH2	7:B:263:SER:O	2.26	0.69
8:C:300:ARG:NH2	22:Q:38:ARG:O	2.26	0.69
9:D:66:SER:O	9:D:72:ASP:OD1	2.10	0.69
15:J:90:GLN:CG	15:J:170:ASP:OD2	2.40	0.69
54:y:7:PHE:CZ	54:y:31:SER:OG	2.45	0.69
1:1:2703:A:OP2	9:D:23:ARG:NH2	2.25	0.69
9:D:165:GLY:O	9:D:168:ASP:HB2	1.92	0.68
44:m:418:ILE:HG13	44:m:419:SER:N	2.07	0.68
6:A:19:HIS:O	6:A:23:ARG:NH1	2.26	0.68
33:b:459:GLU:OE1	52:u:103:ARG:NH2	2.27	0.68
54:y:132:VAL:CG1	54:y:133:LEU:HD12	2.19	0.68
49:r:22:GLU:OE1	49:r:25:ARG:NH2	2.26	0.68
1:1:91:G:OP2	1:1:93:C:N4	2.26	0.68
15:J:143:ARG:O	15:J:144:CYS:CB	2.35	0.68
54:y:132:VAL:HG13	54:y:133:LEU:CD1	2.20	0.68
1:1:2433:U:O2'	19:N:124:ASP:OD1	2.11	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:74:THR:O	4:4:78:GLN:NE2	2.26	0.68
21:P:112:LEU:CD1	21:P:152:GLU:CG	2.72	0.68
1:1:398:A:N6	34:c:88:THR:OG1	2.26	0.68
53:x:473:VAL:O	53:x:476:ARG:NH1	2.27	0.68
1:1:718:G:OP1	32:a:117:ARG:NH2	2.26	0.68
1:1:2737:C:OP1	25:T:70:SER:OG	2.12	0.68
27:V:13:ILE:HD11	27:V:54:LEU:HD12	1.75	0.68
1:1:837:A:OP2	47:p:4:ARG:NH1	2.27	0.68
28:W:145:ARG:NH1	28:W:206:PHE:O	2.27	0.68
33:b:72:ASN:O	33:b:73:ASP:HB2	1.93	0.68
37:f:16:TYR:OH	37:f:89:LEU:O	2.10	0.68
1:1:126:U:OP1	19:N:144:ARG:NH1	2.26	0.67
1:1:364:G:OP2	41:j:52:LYS:NZ	2.25	0.67
3:3:76:A:N3	24:S:50:LYS:NZ	2.43	0.67
51:t:210:ASN:O	51:t:214:GLN:NE2	2.27	0.67
54:y:53:ILE:O	54:y:56:THR:OG1	2.11	0.67
1:1:2891:U:O2'	55:z:2:ALA:N	2.27	0.67
33:b:324:LEU:HD11	33:b:327:ASN:CB	2.23	0.67
1:1:2652:U:OP2	51:t:449:ARG:NH2	2.28	0.67
53:x:136:SER:HB3	53:x:512:LEU:H	1.58	0.67
1:1:937:G:N2	1:1:2813:A:O2'	2.25	0.67
1:1:2397:A:N7	1:1:2981:U:O2	2.28	0.67
3:3:72:A:O2'	3:3:74:C:OP1	2.09	0.67
49:r:208:MET:O	49:r:212:LEU:HD22	1.95	0.67
52:u:116:LYS:O	52:u:119:ASP:OD1	2.12	0.67
4:4:235:ASN:ND2	4:4:326:LEU:O	2.28	0.67
51:t:421:ASN:ND2	51:t:458:ALA:O	2.27	0.67
1:1:2468:A:O3'	1:1:2477:G:N2	2.26	0.67
21:P:47:TYR:OH	21:P:57:ALA:O	2.06	0.67
1:1:1414:G:OP1	34:c:93:ARG:NH2	2.28	0.67
1:1:2878:G:O2'	1:1:2879:C:O5'	2.12	0.66
4:4:531:THR:OG1	4:4:532:CYS:N	2.28	0.66
27:V:36:ILE:HG12	27:V:61:THR:N	2.09	0.66
53:x:364:CYS:SG	53:x:370:SER:CB	2.83	0.66
1:1:3182:G:OP1	20:O:117:ARG:NH2	2.28	0.66
4:4:198:LEU:HD13	4:4:507:ILE:HD11	1.77	0.66
15:J:143:ARG:O	15:J:144:CYS:HB3	1.94	0.66
54:y:7:PHE:CE1	54:y:31:SER:OG	2.48	0.66
1:1:221:A:O2'	1:1:223:U:OP2	2.09	0.66
4:4:475:LEU:HD11	4:4:480:VAL:HG22	1.77	0.66
18:M:36:VAL:HG12	18:M:72:LEU:HD21	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:158:ASP:HB3	12:G:159:PRO:HD3	1.73	0.66
27:V:13:ILE:HD12	27:V:54:LEU:HD12	1.76	0.66
25:T:54:HIS:CD2	25:T:89:LEU:CD2	2.79	0.66
1:1:2661:G:OP1	1:1:2749:G:N2	2.28	0.66
1:1:2964:G:O2'	44:m:31:ARG:NH2	2.29	0.66
4:4:107:GLU:OE1	4:4:420:ARG:NH2	2.28	0.66
4:4:475:LEU:CD1	4:4:480:VAL:HG22	2.26	0.66
6:A:142:ASP:O	6:A:143:GLU:CG	2.40	0.66
8:C:328:ASN:ND2	11:F:182:ASP:OD2	2.29	0.66
27:V:85:TRP:CG	27:V:93:LEU:HD11	2.30	0.66
1:1:2964:G:OP1	44:m:35:ARG:NH2	2.28	0.66
16:K:103:ASP:O	16:K:109:ARG:NH2	2.29	0.66
1:1:2860:U:OP2	33:b:100:ARG:NH2	2.27	0.66
33:b:420:TYR:CE2	33:b:428:LYS:HE2	2.30	0.66
47:p:46:THR:OG1	47:p:57:CYS:SG	2.54	0.66
1:1:210:U:HO2'	1:1:229:G:HO2'	1.33	0.66
9:D:67:SER:HB3	9:D:72:ASP:OD2	1.95	0.66
27:V:36:ILE:CG1	27:V:60:ALA:C	2.69	0.66
33:b:420:TYR:CE2	33:b:428:LYS:CE	2.71	0.66
42:k:32:ASN:C	42:k:33:LYS:NZ	2.53	0.65
21:P:112:LEU:CD1	21:P:152:GLU:HG3	2.26	0.65
37:f:6:ARG:NH1	37:f:8:TYR:O	2.29	0.65
33:b:544:ALA:O	33:b:547:ASP:OD1	2.15	0.65
1:1:877:C:N3	33:b:647:ARG:NH1	2.45	0.65
15:J:10:ARG:NH2	15:J:151:SER:O	2.29	0.65
44:m:96:LEU:HD23	44:m:99:THR:CG2	2.24	0.65
1:1:1188:U:OP1	1:1:1210:U:O2'	2.07	0.65
1:1:2523:A:OP1	29:X:31:THR:OG1	2.14	0.65
33:b:259:GLN:O	33:b:260:CYS:HB3	1.97	0.65
44:m:350:THR:OG1	57:m:501:GTP:O2G	2.13	0.65
7:B:58:ARG:NH2	7:B:352:GLU:OE1	2.29	0.65
16:K:51:ASN:ND2	16:K:53:HIS:O	2.29	0.65
45:n:30:THR:HG22	45:n:91:SER:HB2	1.79	0.65
8:C:325:LEU:O	11:F:41:ARG:NH2	2.29	0.65
4:4:474:PRO:HG2	4:4:475:LEU:HD23	1.79	0.65
15:J:15:GLU:OE2	15:J:72:ARG:NH1	2.29	0.65
33:b:420:TYR:HH	33:b:428:LYS:C	2.05	0.64
17:L:161:ASP:OD1	32:a:139:ARG:NH1	2.31	0.64
51:t:66:GLY:N	51:t:72:MET:O	2.30	0.64
1:1:1493:G:OP2	1:1:1493:G:N2	2.28	0.64
14:I:80:LEU:O	14:I:116:LYS:NZ	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:H:59:ASN:OD1	18:M:41:GLN:NE2	2.29	0.64
54:y:174:SER:OG	54:y:179:VAL:O	2.15	0.64
1:1:1167:U:O2'	11:F:210:PRO:O	2.14	0.64
1:1:1522:U:OP1	29:X:123:TYR:OH	2.15	0.64
1:1:2901:G:O2'	1:1:3024:A:N1	2.31	0.64
1:1:3278:C:OP1	37:f:54:ARG:NH2	2.31	0.64
25:T:26:HIS:O	25:T:29:THR:OG1	2.15	0.64
1:1:1157:G:OP1	11:F:90:LYS:NZ	2.30	0.64
3:3:1:G:O3'	9:D:273:ARG:NH1	2.30	0.64
33:b:497:ARG:NH2	52:u:123:ASP:OD1	2.30	0.64
53:x:156:SER:OG	53:x:500:ARG:NH1	2.31	0.64
1:1:2557:A:OP1	6:A:69:TYR:OH	2.15	0.63
1:1:3175:U:OP1	37:f:10:LYS:NZ	2.30	0.63
53:x:145:THR:O	53:x:164:GLY:N	2.31	0.63
1:1:1899:G:O2'	1:1:2334:U:O4	2.15	0.63
10:E:68:PRO:HG3	10:E:145:LEU:HD23	1.81	0.63
4:4:22:GLU:O	4:4:26:ASN:ND2	2.32	0.63
25:T:54:HIS:CD2	25:T:89:LEU:HD22	2.34	0.63
54:y:128:LEU:O	54:y:132:VAL:HB	1.98	0.63
4:4:66:LEU:HD13	4:4:108:ILE:HD11	1.80	0.63
17:L:131:LYS:H	17:L:131:LYS:CD	2.11	0.63
18:M:65:LEU:HG	24:S:172:TYR:OH	1.98	0.63
54:y:132:VAL:CG1	54:y:133:LEU:H	2.10	0.63
1:1:209:A:O2'	1:1:211:A:OP2	2.11	0.63
1:1:837:A:OP1	47:p:5:THR:OG1	2.14	0.63
1:1:2420:C:O2'	1:1:2802:A:N3	2.28	0.63
1:1:2838:A:OP1	49:r:66:LYS:NZ	2.31	0.63
25:T:54:HIS:CD2	25:T:57:TYR:CD2	2.87	0.63
18:M:24:LYS:NZ	18:M:61:GLY:O	2.27	0.63
33:b:390:PRO:O	33:b:395:ARG:NH1	2.32	0.63
33:b:30:PRO:O	33:b:49:LYS:NZ	2.32	0.63
1:1:3068:U:OP2	23:R:62:ARG:NH1	2.32	0.63
4:4:328:HIS:O	4:4:329:CYS:HB3	1.99	0.62
27:V:13:ILE:HD11	27:V:54:LEU:CD1	2.28	0.62
27:V:94:TYR:OH	52:u:37:HIS:NE2	2.27	0.62
33:b:546:GLN:NE2	33:b:549:GLN:OE1	2.32	0.62
47:p:42:CYS:SG	47:p:60:CYS:CB	2.87	0.62
53:x:289:GLN:OE1	53:x:360:TYR:OH	2.16	0.62
51:t:26:GLU:O	51:t:29:GLN:NE2	2.33	0.62
1:1:2588:U:OP1	12:G:48:ARG:NH2	2.31	0.62
12:G:158:ASP:OD2	12:G:159:PRO:HD3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:V:85:TRP:CG	27:V:93:LEU:CD1	2.83	0.62
33:b:446:ASP:OD2	33:b:452:LYS:NZ	2.32	0.62
42:k:32:ASN:CB	42:k:33:LYS:HZ3	2.03	0.62
3:3:48:U:O2'	9:D:222:LEU:O	2.17	0.62
51:t:481:ALA:O	51:t:484:SER:OG	2.14	0.62
1:1:41:G:O2'	1:1:42:C:O4'	2.18	0.62
1:1:591:G:N2	1:1:612:U:OP1	2.31	0.62
1:1:3167:A:N7	1:1:3282:U:C4	2.67	0.62
33:b:25:THR:O	33:b:29:THR:OG1	2.17	0.62
47:p:59:CYS:O	47:p:60:CYS:HB3	1.99	0.62
1:1:1277:C:O2'	1:1:1278:A:O5'	2.17	0.62
1:1:1695:U:O2'	1:1:1749:A:N1	2.28	0.62
33:b:259:GLN:O	33:b:260:CYS:CB	2.46	0.62
1:1:3092:C:O2'	27:V:12:ARG:NH2	2.32	0.62
2:2:103:G:OP2	2:2:105:A:O2'	2.16	0.62
27:V:85:TRP:CD1	27:V:93:LEU:CD1	2.83	0.62
44:m:245:TYR:HD1	44:m:249:GLU:OE2	1.83	0.62
4:4:247:ILE:HD11	4:4:318:LEU:HB2	1.81	0.61
9:D:36:LEU:O	9:D:48:LYS:NZ	2.31	0.61
12:G:128:LYS:NZ	12:G:202:GLU:OE2	2.34	0.61
1:1:297:G:O2'	40:i:31:GLY:O	2.09	0.61
1:1:929:A:OP1	8:C:61:SER:OG	2.14	0.61
5:5:43:SER:C	5:5:46:LEU:HD23	2.25	0.61
21:P:112:LEU:CD1	21:P:152:GLU:HG2	2.29	0.61
1:1:520:U:O4	8:C:349:THR:OG1	2.18	0.61
1:1:1481:A:O2'	1:1:1859:A:OP2	2.16	0.61
4:4:452:THR:O	4:4:484:LYS:NZ	2.33	0.61
34:c:90:SER:O	34:c:93:ARG:N	2.32	0.61
3:3:38:U:N3	3:3:41:G:OP2	2.33	0.61
21:P:29:THR:HG23	21:P:119:VAL:HG11	1.83	0.61
1:1:1062:A:N3	25:T:130:ARG:NH2	2.48	0.61
19:N:44:ARG:NH1	19:N:120:TRP:O	2.34	0.61
33:b:420:TYR:OH	33:b:428:LYS:O	2.17	0.61
1:1:2323:G:O2'	1:1:2325:G:OP2	2.17	0.60
9:D:38:THR:O	9:D:48:LYS:NZ	2.32	0.60
33:b:305:LEU:O	33:b:308:SER:HB2	2.01	0.60
1:1:1447:G:N7	21:P:25:SER:OG	2.32	0.60
4:4:221:GLN:O	4:4:225:THR:OG1	2.19	0.60
33:b:172:ILE:HG22	33:b:180:LYS:HB2	1.83	0.60
42:k:32:ASN:CB	42:k:33:LYS:HZ1	2.06	0.60
44:m:47:GLU:OE2	44:m:49:ARG:NH2	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:F:29:GLU:OE1	11:F:29:GLU:N	2.35	0.60
12:G:144:GLU:HA	12:G:173:MET:HE2	1.82	0.60
14:I:14:ARG:NH2	14:I:17:ASP:OD2	2.34	0.60
27:V:36:ILE:CG1	27:V:61:THR:N	2.64	0.60
44:m:423:ASP:O	44:m:426:GLU:N	2.33	0.60
1:1:784:A:O2'	22:Q:92:ARG:NH1	2.34	0.60
1:1:2675:C:OP2	1:1:2676:A:O2'	2.16	0.60
1:1:3048:A:OP2	7:B:222:LYS:NZ	2.26	0.60
27:V:36:ILE:HG22	27:V:37:ILE:H	1.65	0.60
31:Z:81:LEU:HD22	38:g:90:ILE:HD13	1.83	0.60
1:1:901:G:OP1	41:j:13:ASN:ND2	2.33	0.60
1:1:2966:G:O6	44:m:31:ARG:NH2	2.34	0.60
3:3:96:U:OP1	24:S:43:TYR:OH	2.13	0.60
21:P:112:LEU:HD11	21:P:152:GLU:HG3	1.84	0.60
27:V:36:ILE:CG1	27:V:60:ALA:HA	2.21	0.60
1:1:1334:U:O2'	11:F:151:ARG:NH2	2.33	0.60
1:1:2940:A:N7	7:B:2:SER:N	2.49	0.60
54:y:199:VAL:HG23	54:y:204:ALA:HB2	1.83	0.60
9:D:62:CYS:SG	9:D:101:THR:HG22	2.42	0.60
12:G:184:ALA:O	12:G:188:THR:HG23	2.02	0.60
25:T:54:HIS:CB	25:T:57:TYR:HB2	2.30	0.60
34:c:89:LEU:HD23	34:c:89:LEU:O	2.02	0.60
1:1:714:G:N7	32:a:111:LYS:NZ	2.42	0.60
6:A:142:ASP:C	6:A:143:GLU:HG3	2.27	0.60
11:F:154:GLY:O	11:F:161:VAL:N	2.35	0.60
22:Q:22:ASP:N	22:Q:22:ASP:OD1	2.34	0.60
1:1:3276:G:O6	21:P:171:ARG:NH1	2.34	0.59
52:u:119:ASP:OD1	52:u:120:PHE:N	2.34	0.59
1:1:148:G:OP2	19:N:4:TYR:OH	2.13	0.59
1:1:3215:A:H5'	18:M:121:MET:HE1	1.84	0.59
1:1:436:A:OP2	1:1:621:A:N6	2.32	0.59
1:1:2929:C:O2'	1:1:2930:A:O4'	2.20	0.59
10:E:60:ASP:OD1	10:E:62:THR:OG1	2.16	0.59
33:b:420:TYR:OH	33:b:428:LYS:C	2.44	0.59
1:1:3004:C:OP2	7:B:28:ARG:NH2	2.36	0.59
15:J:141:ARG:NH2	15:J:144:CYS:SG	2.75	0.59
16:K:80:SER:O	16:K:84:ILE:HG22	2.02	0.59
53:x:207:ASP:OD2	53:x:209:THR:OG1	2.15	0.59
1:1:198:A:N3	1:1:218:G:O2'	2.33	0.59
1:1:971:G:OP1	22:Q:8:LYS:NZ	2.27	0.59
1:1:3041:U:OP1	27:V:12:ARG:NH1	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:140:LYS:NZ	4:4:500:VAL:O	2.21	0.59
1:1:2137:U:OP2	1:1:2142:A:N6	2.36	0.59
1:1:2370:G:OP1	50:s:12:SER:HB2	2.02	0.59
4:4:475:LEU:CG	4:4:480:VAL:HG22	2.32	0.59
1:1:1197:A:O2'	3:3:89:G:OP2	2.20	0.59
1:1:2715:A:N7	51:t:504:LYS:NZ	2.51	0.59
4:4:94:THR:HB	4:4:142:THR:HG23	1.85	0.59
33:b:70:ASN:O	33:b:74:VAL:HG13	2.03	0.59
53:x:401:HIS:NE2	53:x:419:SER:OG	2.18	0.59
17:L:131:LYS:HE2	17:L:131:LYS:N	2.17	0.59
27:V:76:ALA:HB1	27:V:101:VAL:O	2.03	0.59
48:q:54:LYS:HE2	48:q:58:VAL:HG11	1.85	0.59
1:1:1722:U:OP1	23:R:100:ARG:NH1	2.34	0.59
1:1:912:G:OP2	6:A:9:ARG:NH1	2.34	0.58
1:1:689:U:O4	8:C:209:TYR:OH	2.18	0.58
4:4:274:GLN:HE22	4:4:335:VAL:HG12	1.67	0.58
39:h:84:LYS:O	39:h:85:THR:HG23	2.03	0.58
45:n:34:LEU:HD23	45:n:59:TYR:HB3	1.83	0.58
1:1:1222:G:N7	28:W:71:LYS:NZ	2.42	0.58
2:2:135:G:OP2	29:X:56:ARG:NH2	2.37	0.58
4:4:488:LEU:HA	4:4:491:SER:OG	2.03	0.58
10:E:40:LEU:HD13	10:E:84:VAL:HG11	1.84	0.58
31:Z:33:SER:CB	31:Z:35:SER:O	2.52	0.58
1:1:769:G:O2'	17:L:168:ARG:NH2	2.34	0.58
17:L:161:ASP:OD2	32:a:139:ARG:NH2	2.37	0.58
21:P:127:ARG:HH21	21:P:139:TYR:HD2	1.51	0.58
1:1:1481:A:N3	1:1:1858:A:O2'	2.36	0.58
1:1:1559:A:OP1	29:X:33:ARG:NE	2.37	0.58
1:1:2725:U:O2'	1:1:2731:U:O4	2.21	0.58
1:1:3167:A:N7	1:1:3282:U:O4	2.37	0.58
9:D:86:TYR:OH	9:D:250:ASP:O	2.17	0.58
15:J:30:LEU:HD22	15:J:64:LYS:O	2.02	0.58
12:G:160:ILE:O	12:G:164:VAL:HG13	2.03	0.58
34:c:138:SER:O	34:c:141:THR:OG1	2.15	0.58
8:C:289:ILE:HG23	22:Q:129:VAL:HG12	1.86	0.58
27:V:13:ILE:CG1	27:V:54:LEU:HD13	2.31	0.58
1:1:1888:U:OP1	7:B:247:ARG:NH1	2.37	0.57
15:J:84:LEU:HD11	15:J:91:LEU:HD21	1.85	0.57
44:m:248:LYS:HB2	44:m:249:GLU:OE1	2.04	0.57
1:1:1111:U:O2'	1:1:1112:A:O5'	2.15	0.57
21:P:8:SER:HB2	34:c:85:THR:OG1	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2989:U:O2'	7:B:267:ALA:O	2.20	0.57
21:P:108:ASP:OD2	21:P:110:THR:OG1	2.23	0.57
21:P:112:LEU:HD12	21:P:152:GLU:CG	2.33	0.57
25:T:41:ASP:OD2	25:T:61:THR:HG22	2.04	0.57
38:g:44:CYS:CB	38:g:81:CYS:SG	2.93	0.57
42:k:32:ASN:C	42:k:33:LYS:HZ1	2.12	0.57
15:J:117:ASP:OD1	15:J:119:SER:CB	2.52	0.57
39:h:38:ARG:NH2	39:h:40:SER:OG	2.38	0.57
1:1:1355:A:OP1	10:E:8:LYS:NZ	2.34	0.57
7:B:251:CYS:SG	7:B:253:GLY:N	2.78	0.57
33:b:268:VAL:HG21	33:b:305:LEU:HD22	1.86	0.57
3:3:6:C:OP2	9:D:22:ARG:NH1	2.38	0.57
8:C:304:GLN:NE2	8:C:306:THR:O	2.38	0.57
51:t:31:GLU:OE1	51:t:31:GLU:N	2.38	0.57
1:1:1634:G:N7	31:Z:17:ARG:NH1	2.53	0.57
1:1:2722:U:P	25:T:88:ARG:NH1	2.78	0.56
31:Z:33:SER:HB3	31:Z:35:SER:O	2.05	0.56
38:g:11:ASN:O	38:g:18:ASN:ND2	2.38	0.56
52:u:32:CYS:SG	52:u:33:ARG:NH2	2.77	0.56
1:1:2253:G:OP1	51:t:177:ARG:NH2	2.39	0.56
7:B:297:SER:OG	33:b:431:ILE:HD11	2.05	0.56
33:b:324:LEU:HD13	33:b:327:ASN:H	1.70	0.56
44:m:160:LEU:O	44:m:164:THR:HG23	2.06	0.56
4:4:108:ILE:HD12	4:4:108:ILE:H	1.70	0.56
4:4:347:SER:OG	4:4:352:GLU:OE1	2.22	0.56
9:D:148:ILE:HD11	9:D:159:VAL:HG21	1.87	0.56
11:F:112:ASN:ND2	11:F:209:ASN:OD1	2.39	0.56
15:J:25:GLU:OE1	15:J:29:ARG:NH1	2.39	0.56
51:t:386:TYR:OH	51:t:410:ALA:O	2.19	0.56
16:K:209:THR:O	16:K:213:ASN:ND2	2.38	0.56
1:1:1597:C:OP1	38:g:31:ARG:NH1	2.38	0.56
1:1:2179:C:O2'	6:A:174:ARG:NH2	2.38	0.56
53:x:449:GLN:N	53:x:462:CYS:SG	2.78	0.56
54:y:186:VAL:HG23	54:y:193:VAL:HG12	1.86	0.56
1:1:216:G:OP1	30:Y:16:ARG:NH1	2.37	0.56
1:1:2547:A:OP1	6:A:93:LYS:NZ	2.32	0.56
1:1:2844:C:O2'	1:1:2845:A:O3'	2.24	0.56
45:n:40:LYS:HB3	45:n:101:LEU:HD21	1.88	0.56
54:y:73:PRO:O	54:y:76:THR:OG1	2.20	0.56
4:4:475:LEU:HG	4:4:480:VAL:HG22	1.87	0.56
1:1:576:C:OP1	11:F:241:LYS:NZ	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2673:A:O2'	15:J:126:ASP:OD1	2.12	0.56
1:1:2831:G:N3	49:r:256:ASN:ND2	2.54	0.56
12:G:134:TYR:CG	12:G:190:VAL:HG21	2.41	0.56
17:L:57:VAL:HG22	17:L:69:VAL:HG22	1.88	0.56
1:1:1603:A:OP1	23:R:38:ARG:NH1	2.38	0.56
1:1:1868:G:HO2'	1:1:2118:C:HO2'	1.40	0.56
3:3:121:U:O4	9:D:264:GLN:NE2	2.39	0.56
4:4:272:SER:OG	4:4:474:PRO:O	2.23	0.56
1:1:642:U:O2'	1:1:643:U:O5'	2.22	0.55
4:4:462:ALA:HB3	33:b:594:ALA:O	2.06	0.55
16:K:297:ILE:CG2	16:K:298:GLU:N	2.69	0.55
21:P:118:GLN:OE1	21:P:120:ASN:ND2	2.39	0.55
1:1:1200:A:OP1	50:s:26:HIS:NE2	2.39	0.55
11:F:151:ARG:NE	11:F:206:LYS:O	2.39	0.55
1:1:2711:C:O2'	1:1:2744:U:OP1	2.24	0.55
48:q:143:VAL:HG13	48:q:151:ILE:HD12	1.88	0.55
15:J:112:LEU:HD12	15:J:112:LEU:O	2.07	0.55
26:U:94:ARG:HE	26:U:96:VAL:CG1	2.20	0.55
4:4:224:ARG:NH2	4:4:268:VAL:O	2.40	0.55
13:H:21:LYS:HG2	13:H:22:SER:H	1.71	0.55
24:S:170:THR:HG23	24:S:170:THR:O	2.06	0.55
53:x:411:SER:OG	53:x:413:ASP:OD1	2.18	0.55
54:y:120:ASP:O	54:y:139:ARG:NH1	2.38	0.55
30:Y:91:ASN:OD1	30:Y:93:ALA:N	2.39	0.55
4:4:20:LEU:HD21	4:4:508:VAL:HG22	1.88	0.55
9:D:218:ARG:NH1	9:D:221:GLU:OE2	2.40	0.55
4:4:148:ASP:OD2	4:4:249:ARG:NH1	2.40	0.55
33:b:380:GLU:O	33:b:384:ASN:ND2	2.40	0.55
1:1:200:C:OP2	30:Y:60:ARG:NH1	2.40	0.54
1:1:2937:G:O2'	33:b:28:LYS:O	2.23	0.54
14:I:7:LYS:O	14:I:13:ARG:NH1	2.40	0.54
25:T:103:GLN:NE2	25:T:104:GLU:HB2	2.21	0.54
44:m:418:ILE:CG1	44:m:419:SER:N	2.69	0.54
51:t:18:GLN:NE2	51:t:96:GLN:OE1	2.39	0.54
51:t:200:LEU:O	51:t:204:THR:HG22	2.07	0.54
14:I:16:ARG:NH1	14:I:24:ASP:OD2	2.38	0.54
17:L:43:ALA:O	17:L:47:ALA:HA	2.07	0.54
1:1:1680:G:OP2	26:U:90:ARG:NH2	2.41	0.54
51:t:385:ILE:HG23	51:t:386:TYR:CG	2.43	0.54
1:1:1145:G:O2'	36:e:45:ARG:O	2.21	0.54
4:4:122:ASP:OD1	4:4:124:THR:HG22	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:274:GLN:NE2	4:4:335:VAL:HG12	2.23	0.54
44:m:245:TYR:CD1	44:m:249:GLU:CD	2.85	0.54
51:t:252:ASP:HB3	51:t:255:ILE:HD12	1.89	0.54
1:1:2272:G:OP1	44:m:297:GLY:N	2.39	0.54
1:1:2383:C:OP2	20:O:85:ARG:NH2	2.39	0.54
44:m:245:TYR:CE1	44:m:249:GLU:CG	2.87	0.54
1:1:2652:U:O2'	1:1:2653:C:OP2	2.17	0.54
15:J:133:ARG:NH2	15:J:158:ASP:OD1	2.41	0.54
31:Z:53:VAL:HG21	31:Z:62:VAL:CG2	2.37	0.54
48:q:161:GLU:O	48:q:162:ILE:HD13	2.08	0.54
4:4:325:SER:O	4:4:326:LEU:HD23	2.07	0.54
16:K:69:VAL:O	16:K:73:THR:OG1	2.23	0.54
22:Q:36:LEU:O	22:Q:40:THR:OG1	2.15	0.54
33:b:177:ASN:OD1	33:b:197:TYR:O	2.26	0.54
1:1:2320:A:H2	47:p:16:VAL:HG12	1.73	0.54
1:1:3217:C:O2'	1:1:3218:A:O5'	2.26	0.54
33:b:74:VAL:HG23	33:b:75:HIS:H	1.71	0.54
33:b:320:SER:OG	33:b:327:ASN:HB3	2.08	0.54
54:y:206:THR:OG1	54:y:207:GLY:N	2.41	0.54
7:B:58:ARG:NH1	7:B:283:TYR:OH	2.41	0.53
38:g:38:LEU:O	38:g:58:ARG:NH2	2.41	0.53
1:1:408:A:N3	1:1:655:C:O2'	2.38	0.53
4:4:363:ASP:HB2	33:b:573:LEU:HD13	1.89	0.53
1:1:2125:A:O2'	44:m:452:GLN:OE1	2.17	0.53
11:F:110:ARG:O	11:F:113:SER:OG	2.25	0.53
25:T:53:PRO:CB	25:T:54:HIS:HD1	2.21	0.53
38:g:74:ARG:CZ	38:g:82:ALA:HB2	2.38	0.53
53:x:365:LYS:HD3	53:x:370:SER:HB2	1.91	0.53
9:D:215:ASP:OD1	9:D:216:GLU:N	2.41	0.53
33:b:542:MET:SD	33:b:542:MET:N	2.81	0.53
4:4:157:THR:OG1	4:4:502:ARG:O	2.23	0.53
8:C:338:LYS:O	8:C:340:GLY:N	2.41	0.53
10:E:53:VAL:HG11	10:E:145:LEU:HD21	1.90	0.53
23:R:13:SER:OG	23:R:38:ARG:NH2	2.41	0.53
23:R:130:ASN:O	23:R:131:ALA:HB3	2.09	0.53
25:T:54:HIS:NE2	25:T:89:LEU:CD1	2.71	0.53
53:x:382:THR:HG21	53:x:397:ARG:HE	1.73	0.53
55:z:23:GLN:O	55:z:26:VAL:HG12	2.09	0.53
15:J:14:ILE:HG13	15:J:131:MET:HE1	1.90	0.53
17:L:165:SER:O	17:L:168:ARG:N	2.41	0.53
42:k:58:ASP:OD2	42:k:61:LYS:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:t:355:THR:HG22	51:t:355:THR:O	2.09	0.53
4:4:378:LEU:HD13	4:4:419:PHE:CD1	2.44	0.53
14:I:26:SER:O	14:I:119:ASN:ND2	2.42	0.53
25:T:54:HIS:CD2	25:T:89:LEU:HD21	2.41	0.53
1:1:1214:U:OP2	24:S:137:ARG:NH2	2.42	0.53
25:T:68:THR:OG1	25:T:71:SER:OG	1.93	0.53
54:y:132:VAL:HG12	54:y:133:LEU:H	1.74	0.53
7:B:287:LYS:HB3	7:B:289:ASP:OD1	2.09	0.52
34:c:109:LEU:CA	34:c:112:ASP:OD2	2.36	0.52
44:m:418:ILE:HG13	44:m:419:SER:H	1.73	0.52
54:y:199:VAL:HG23	54:y:204:ALA:CB	2.39	0.52
55:z:23:GLN:HA	55:z:26:VAL:HG12	1.89	0.52
1:1:363:G:OP2	41:j:56:ARG:NH2	2.42	0.52
4:4:543:LEU:HD23	4:4:554:PHE:CZ	2.44	0.52
7:B:187:SER:O	7:B:190:GLU:N	2.41	0.52
15:J:32:ARG:O	15:J:36:VAL:HG23	2.10	0.52
27:V:85:TRP:CD2	27:V:93:LEU:CD1	2.87	0.52
34:c:46:LYS:NZ	34:c:56:ASP:OD1	2.41	0.52
38:g:100:ILE:O	38:g:104:VAL:HG13	2.10	0.52
48:q:58:VAL:HG12	48:q:79:SER:HB2	1.91	0.52
9:D:66:SER:C	9:D:72:ASP:OD1	2.53	0.52
35:d:33:VAL:HG13	35:d:51:LEU:HD11	1.91	0.52
49:r:185:THR:HB	49:r:192:THR:HG22	1.91	0.52
5:5:42:THR:OG1	5:5:45:GLU:CB	2.48	0.52
16:K:297:ILE:HG23	16:K:298:GLU:N	2.23	0.52
27:V:13:ILE:CD1	27:V:54:LEU:HD13	2.40	0.52
53:x:494:TRP:HA	53:x:501:VAL:HG12	1.92	0.52
1:1:2737:C:H4'	25:T:68:THR:HG21	1.92	0.52
9:D:217:GLU:N	9:D:217:GLU:OE2	2.43	0.52
7:B:10:ARG:NH1	7:B:11:HIS:O	2.42	0.52
9:D:99:TYR:HE1	9:D:168:ASP:OD1	1.90	0.52
29:X:5:ALA:O	29:X:8:THR:HB	2.10	0.52
28:W:96:CYS:HB3	28:W:100:THR:HG21	1.91	0.52
31:Z:81:LEU:HD22	38:g:90:ILE:CD1	2.40	0.52
44:m:312:ASP:OD1	44:m:313:ARG:NH1	2.43	0.52
49:r:214:VAL:HG12	49:r:216:THR:HG23	1.92	0.52
1:1:3165:A:H62	1:1:3285:C:H41	1.57	0.52
4:4:475:LEU:HD21	4:4:480:VAL:CG2	2.40	0.52
28:W:123:ASP:OD1	28:W:124:TYR:N	2.40	0.52
4:4:20:LEU:HD21	4:4:508:VAL:CG2	2.40	0.52
4:4:41:TYR:O	4:4:44:SER:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:R:95:TRP:HZ3	23:R:130:ASN:OD1	1.89	0.52
53:x:188:TRP:O	53:x:206:MET:N	2.43	0.52
54:y:103:ALA:O	54:y:107:VAL:HG23	2.10	0.52
16:K:294:ALA:C	16:K:297:ILE:HG22	2.33	0.51
33:b:172:ILE:HD13	33:b:183:PHE:HD2	1.75	0.51
54:y:207:GLY:O	54:y:210:THR:HG22	2.11	0.51
1:1:1241:U:O2'	1:1:1242:G:O5'	2.21	0.51
8:C:36:HIS:O	8:C:40:THR:HG23	2.10	0.51
25:T:105:PHE:O	25:T:109:VAL:HG23	2.11	0.51
34:c:148:TRP:CE3	34:c:151:ILE:HD11	2.46	0.51
35:d:16:LEU:HD11	35:d:71:LEU:HD12	1.92	0.51
1:1:2857:C:O4'	49:r:192:THR:OG1	2.27	0.51
28:W:38:ARG:NE	28:W:224:ASP:OD2	2.44	0.51
42:k:17:ARG:NH2	42:k:19:ASP:OD2	2.42	0.51
25:T:53:PRO:CB	25:T:54:HIS:ND1	2.74	0.51
8:C:302:ALA:HB2	22:Q:39:ARG:NH1	2.25	0.51
44:m:227:HIS:NE2	44:m:238:ARG:O	2.43	0.51
1:1:1229:G:O3'	28:W:126:ARG:NH1	2.43	0.51
1:1:3340:G:O2'	1:1:3341:U:O4'	2.23	0.51
2:2:123:G:O2'	2:2:124:G:OP1	2.23	0.51
4:4:151:THR:HG21	4:4:252:ALA:HB2	1.91	0.51
16:K:307:LYS:HA	16:K:310:VAL:HG13	1.93	0.51
39:h:77:PRO:HD2	39:h:80:LEU:HD12	1.91	0.51
48:q:76:SER:OG	48:q:79:SER:OG	2.09	0.51
2:2:12:A:OP1	21:P:3:ARG:NH2	2.43	0.51
4:4:223:ILE:O	4:4:227:VAL:HG12	2.10	0.51
33:b:43:ARG:NH2	33:b:119:GLY:O	2.43	0.51
54:y:63:THR:CG2	54:y:72:VAL:HG12	2.41	0.51
54:y:143:SER:O	54:y:143:SER:OG	2.28	0.51
1:1:1307:G:O2'	1:1:1308:A:OP2	2.26	0.51
1:1:2851:A:N3	49:r:55:TYR:OH	2.37	0.51
4:4:466:LEU:C	4:4:467:THR:CG2	2.80	0.51
17:L:47:ALA:HB3	17:L:48:PRO:HD3	1.93	0.51
23:R:115:ILE:HD11	23:R:119:LEU:HG	1.92	0.51
33:b:324:LEU:HD12	33:b:324:LEU:C	2.36	0.51
1:1:1471:U:OP1	23:R:5:ARG:NH2	2.44	0.51
12:G:78:PHE:O	12:G:79:GLN:CG	2.50	0.51
16:K:84:ILE:HD11	16:K:89:LEU:CB	2.41	0.51
21:P:112:LEU:HD12	21:P:152:GLU:HG2	1.92	0.51
51:t:385:ILE:HG23	51:t:386:TYR:N	2.26	0.51
51:t:385:ILE:CG2	51:t:386:TYR:CD2	2.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:J:90:GLN:HB3	15:J:172:LEU:HD11	1.92	0.50
37:f:49:ILE:HD11	37:f:71:VAL:HG22	1.92	0.50
4:4:227:VAL:HG11	4:4:269:TRP:CZ2	2.45	0.50
12:G:223:ALA:O	12:G:227:ASP:N	2.44	0.50
13:H:21:LYS:CG	13:H:22:SER:H	2.24	0.50
27:V:85:TRP:CE2	27:V:93:LEU:HD11	2.45	0.50
33:b:506:GLU:HA	35:d:97:LEU:HD13	1.93	0.50
54:y:160:LEU:HD12	54:y:182:VAL:O	2.11	0.50
1:1:1142:G:O6	1:1:1143:A:N6	2.44	0.50
1:1:2680:A:OP1	15:J:51:ARG:NH1	2.45	0.50
27:V:13:ILE:HG22	27:V:85:TRP:HB3	1.94	0.50
1:1:195:U:O2'	34:c:103:TYR:OH	2.22	0.50
1:1:1900:A:O2'	1:1:1906:G:N7	2.36	0.50
40:i:66:GLU:N	40:i:66:GLU:OE2	2.44	0.50
1:1:3109:G:OP1	49:r:23:ARG:NH1	2.44	0.50
4:4:261:GLU:OE1	4:4:261:GLU:HA	2.12	0.50
38:g:44:CYS:HB2	38:g:81:CYS:SG	2.52	0.50
1:1:645:A:O2'	1:1:647:A:N7	2.30	0.50
1:1:1010:G:O6	53:x:427:LYS:NZ	2.44	0.50
17:L:123:ILE:HG22	39:h:118:ILE:HG22	1.94	0.50
22:Q:40:THR:O	22:Q:41:ASP:OD1	2.30	0.50
27:V:118:VAL:HG12	27:V:135:VAL:O	2.12	0.50
33:b:254:MET:O	33:b:267:GLN:NE2	2.44	0.50
53:x:254:SER:OG	53:x:255:SER:N	2.45	0.50
53:x:377:ALA:HB1	53:x:405:VAL:HB	1.93	0.50
1:1:952:A:N3	1:1:1114:U:O2'	2.42	0.50
7:B:251:CYS:SG	7:B:252:ILE:N	2.84	0.50
14:I:88:GLU:N	14:I:88:GLU:OE1	2.43	0.50
27:V:76:ALA:HB2	27:V:103:ALA:N	2.27	0.50
33:b:318:MET:HE1	33:b:330:GLU:OE2	2.12	0.50
44:m:249:GLU:OE1	44:m:249:GLU:N	2.44	0.50
1:1:68:C:OP2	1:1:301:G:N2	2.45	0.50
1:1:562:C:OP2	18:M:77:ARG:NH1	2.43	0.50
1:1:1863:G:N1	1:1:1866:C:OP2	2.43	0.50
1:1:2568:C:O2'	1:1:2569:A:O5'	2.27	0.50
1:1:2841:G:O2'	1:1:2842:U:OP2	2.27	0.50
1:1:3275:U:O2'	37:f:99:ARG:NH1	2.45	0.50
9:D:182:GLY:HA3	9:D:194:LEU:HD23	1.93	0.50
22:Q:123:THR:OG1	22:Q:125:ASP:OD1	2.26	0.50
24:S:77:VAL:HG21	24:S:106:LEU:CD1	2.42	0.50
27:V:83:LYS:NZ	27:V:84:SER:OG	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:b:177:ASN:OD1	33:b:197:TYR:N	2.44	0.50
1:1:86:G:O2'	1:1:98:G:O6	2.29	0.49
1:1:1200:A:H2	1:1:2824:G:H22	1.60	0.49
1:1:2461:A:O2'	1:1:2463:G:OP2	2.30	0.49
4:4:203:THR:OG1	4:4:205:GLU:O	2.28	0.49
4:4:262:ARG:NH1	33:b:569:ASP:OD2	2.44	0.49
15:J:31:THR:C	15:J:34:SER:HB3	2.34	0.49
25:T:54:HIS:HE1	25:T:89:LEU:HD11	1.77	0.49
45:n:44:ILE:CG2	45:n:48:THR:HG21	2.42	0.49
4:4:227:VAL:HG21	4:4:321:LEU:HD11	1.94	0.49
27:V:36:ILE:HG12	27:V:61:THR:H	1.77	0.49
33:b:398:LEU:HD22	54:y:39:GLU:CB	2.33	0.49
45:n:34:LEU:HD23	45:n:59:TYR:CB	2.42	0.49
1:1:2177:G:OP2	6:A:128:ARG:NH1	2.46	0.49
1:1:3039:C:O2'	27:V:10:LYS:O	2.21	0.49
12:G:228:GLU:OE2	12:G:232:HIS:HD2	1.95	0.49
13:H:120:ASP:OD2	13:H:124:ARG:NH1	2.45	0.49
27:V:23:MET:HE3	27:V:100:GLY:HA2	1.95	0.49
16:K:294:ALA:HA	16:K:297:ILE:CG2	2.42	0.49
1:1:1681:U:OP2	33:b:521:ARG:NH2	2.46	0.49
13:H:31:ARG:HD2	13:H:149:ASN:OD1	2.13	0.49
44:m:155:SER:OG	44:m:156:ASN:N	2.45	0.49
53:x:305:ASP:OD2	53:x:308:SER:OG	2.16	0.49
1:1:2316:G:O2'	44:m:292:ASN:OD1	2.24	0.49
3:3:12:U:OP2	3:3:68:C:O2'	2.30	0.49
22:Q:134:GLY:O	22:Q:137:THR:OG1	2.23	0.49
34:c:57:LEU:O	34:c:61:ASN:OD1	2.31	0.49
53:x:264:ASP:O	53:x:268:ARG:N	2.46	0.49
10:E:93:VAL:HG13	10:E:96:VAL:HG22	1.95	0.49
52:u:126:LEU:C	52:u:129:SER:HG	2.10	0.49
1:1:196:G:N1	1:1:199:A:OP2	2.44	0.49
1:1:395:A:O3'	34:c:95:LYS:NZ	2.42	0.49
1:1:640:U:O2'	1:1:941:G:OP2	2.23	0.49
9:D:164:LYS:O	9:D:168:ASP:CG	2.56	0.49
1:1:3085:G:OP1	52:u:34:SER:OG	2.28	0.49
7:B:289:ASP:OD1	7:B:289:ASP:N	2.46	0.49
14:I:74:LYS:HA	14:I:77:VAL:HG22	1.94	0.49
15:J:117:ASP:OD1	15:J:119:SER:HB3	2.13	0.49
20:O:103:LYS:NZ	34:c:8:ASN:O	2.44	0.49
33:b:183:PHE:HA	33:b:186:CYS:SG	2.52	0.49
51:t:213:ASP:OD2	51:t:214:GLN:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:97:ILE:HG22	4:4:137:ASP:OD1	2.13	0.49
16:K:307:LYS:HA	16:K:310:VAL:CG1	2.43	0.49
32:a:85:ASP:OD2	32:a:86:LYS:N	2.46	0.49
33:b:324:LEU:CD1	33:b:327:ASN:CB	2.91	0.49
34:c:89:LEU:HD22	34:c:94:ALA:HB2	1.95	0.49
1:1:835:G:O2'	1:1:857:G:N2	2.36	0.48
1:1:2722:U:C5'	25:T:88:ARG:CZ	2.91	0.48
1:1:3172:A:OP1	55:z:100:LYS:NZ	2.45	0.48
4:4:238:VAL:HG11	4:4:269:TRP:HB3	1.95	0.48
15:J:54:VAL:O	51:t:434:ASP:OD1	2.31	0.48
18:M:59:ASN:OD1	18:M:60:LEU:N	2.46	0.48
33:b:79:ARG:NH1	44:m:167:ASP:OD2	2.43	0.48
44:m:245:TYR:CD1	44:m:249:GLU:OE2	2.65	0.48
51:t:101:PHE:O	51:t:105:THR:OG1	2.22	0.48
1:1:28:C:O2'	1:1:61:A:N3	2.41	0.48
1:1:1382:G:OP2	8:C:188:ARG:NH1	2.46	0.48
1:1:2522:G:O2'	1:1:2524:A:OP2	2.28	0.48
26:U:21:SER:HB3	26:U:22:PRO:HD3	1.94	0.48
44:m:63:ASP:OD2	44:m:65:THR:OG1	2.23	0.48
44:m:192:ASN:O	44:m:192:ASN:ND2	2.44	0.48
44:m:277:LEU:HB2	44:m:283:THR:HG21	1.95	0.48
51:t:145:THR:OG1	51:t:147:GLU:OE1	2.27	0.48
1:1:1322:U:O2	24:S:108:GLN:NE2	2.45	0.48
8:C:329:PRO:C	11:F:45:LEU:HD12	2.38	0.48
11:F:87:VAL:HG11	11:F:243:MET:HE1	1.95	0.48
54:y:113:TYR:O	54:y:135:VAL:HG23	2.13	0.48
4:4:178:GLY:O	4:4:182:ASP:OD1	2.31	0.48
19:N:163:GLY:O	19:N:172:ARG:NH1	2.44	0.48
23:R:105:LEU:HD22	23:R:135:LYS:HD3	1.95	0.48
53:x:331:ASP:OD2	53:x:332:TYR:N	2.46	0.48
53:x:430:ASP:OD1	53:x:435:LYS:N	2.43	0.48
4:4:332:LYS:NZ	34:c:153:ASP:O	2.38	0.48
7:B:155:ALA:O	7:B:156:SER:HB3	2.13	0.48
27:V:85:TRP:CE2	27:V:93:LEU:CD1	2.97	0.48
33:b:422:LEU:HD13	33:b:427:TRP:HE1	1.78	0.48
44:m:332:ILE:HG21	44:m:356:ILE:HD13	1.94	0.48
1:1:339:C:OP1	1:1:1380:G:O2'	2.31	0.48
4:4:403:HIS:ND1	4:4:408:GLU:OE2	2.45	0.48
14:I:96:TYR:HE2	33:b:443:ASP:OD2	1.96	0.48
16:K:104:GLU:OE1	16:K:104:GLU:N	2.46	0.48
33:b:184:LEU:HA	33:b:187:ILE:HG22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:b:263:THR:HG23	33:b:266:ALA:H	1.77	0.48
33:b:423:GLU:OE1	33:b:423:GLU:N	2.46	0.48
1:1:1308:A:O2'	1:1:1311:G:OP1	2.19	0.48
1:1:2700:G:N2	1:1:2755:C:N3	2.61	0.48
27:V:32:ARG:HB3	27:V:33:ASN:OD1	2.13	0.48
31:Z:41:ALA:HB2	31:Z:77:TYR:HE1	1.78	0.48
54:y:175:SER:O	54:y:178:GLN:NE2	2.46	0.48
9:D:104:LEU:HD11	9:D:108:ARG:HH21	1.78	0.48
13:H:14:GLU:OE1	13:H:14:GLU:N	2.45	0.48
33:b:417:LYS:O	33:b:418:ASP:HB2	2.14	0.48
1:1:1703:U:O4	1:1:1740:U:O2'	2.23	0.47
1:1:3139:A:OP2	7:B:30:LYS:NZ	2.27	0.47
47:p:75:ALA:O	47:p:79:VAL:HG23	2.13	0.47
1:1:336:A:O2'	8:C:48:GLN:NE2	2.47	0.47
1:1:1920:U:O2'	1:1:1932:A:N7	2.41	0.47
1:1:3153:U:OP2	1:1:3293:U:O2'	2.23	0.47
4:4:475:LEU:CD1	4:4:480:VAL:CG2	2.84	0.47
8:C:237:GLN:O	8:C:246:ARG:NH1	2.43	0.47
27:V:17:LEU:HD21	27:V:98:ASN:OD1	2.14	0.47
33:b:72:ASN:C	33:b:73:ASP:CG	2.81	0.47
38:g:44:CYS:SG	38:g:80:ARG:HA	2.54	0.47
1:1:1480:G:O2'	1:1:1871:U:O4	2.30	0.47
1:1:1678:G:O6	26:U:74:LYS:NZ	2.47	0.47
1:1:3234:A:H2	1:1:3253:G:H22	1.62	0.47
9:D:236:LEU:HD12	9:D:237:GLU:N	2.30	0.47
23:R:95:TRP:CE3	23:R:98:ARG:CZ	2.96	0.47
33:b:460:GLU:OE2	52:u:103:ARG:NE	2.45	0.47
1:1:1063:G:C6	25:T:109:VAL:HG22	2.50	0.47
4:4:159:VAL:CG1	4:4:535:SER:CB	2.93	0.47
27:V:85:TRP:NE1	27:V:93:LEU:HD12	2.29	0.47
9:D:236:LEU:HA	9:D:239:ILE:HD12	1.96	0.47
11:F:82:LYS:O	11:F:119:VAL:HG12	2.14	0.47
22:Q:64:VAL:HG13	22:Q:96:PHE:CE1	2.49	0.47
27:V:36:ILE:HG22	27:V:37:ILE:HG13	1.96	0.47
27:V:36:ILE:HD11	27:V:61:THR:HG23	1.97	0.47
30:Y:88:GLU:HG3	34:c:140:LEU:HD23	1.96	0.47
12:G:74:THR:O	12:G:77:GLN:NE2	2.48	0.47
12:G:146:LYS:HE3	12:G:173:MET:HE3	1.95	0.47
54:y:16:PHE:HD1	54:y:27:ALA:HB3	1.79	0.47
6:A:113:VAL:HG12	6:A:166:ILE:HD13	1.97	0.47
12:G:75:ILE:HD12	19:N:18:VAL:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:V:130:ALA:O	54:y:106:ASN:ND2	2.47	0.47
51:t:491:ASP:OD2	51:t:491:ASP:N	2.47	0.47
53:x:179:MET:O	53:x:180:HIS:C	2.56	0.47
55:z:4:SER:OG	55:z:5:LEU:N	2.46	0.47
1:1:2385:G:O6	34:c:11:LYS:NZ	2.48	0.47
1:1:2466:G:N2	46:o:209:SER:O	2.42	0.47
27:V:76:ALA:CB	27:V:102:ILE:HA	2.44	0.47
32:a:120:ASN:ND2	32:a:120:ASN:O	2.46	0.47
47:p:60:CYS:SG	47:p:62:LYS:HG3	2.55	0.47
53:x:156:SER:HG	53:x:500:ARG:HH11	1.63	0.47
54:y:132:VAL:CG1	54:y:133:LEU:CD1	2.87	0.47
1:1:2722:U:H5'	25:T:88:ARG:CZ	2.44	0.47
4:4:26:ASN:O	4:4:30:THR:HG22	2.15	0.47
4:4:338:GLU:HB3	4:4:489:MET:HE1	1.97	0.47
55:z:15:SER:O	55:z:19:ARG:NE	2.37	0.47
15:J:141:ARG:NE	15:J:144:CYS:HB3	2.29	0.46
32:a:83:PRO:HB2	32:a:85:ASP:OD2	2.14	0.46
1:1:213:A:N6	1:1:227:G:O2'	2.48	0.46
1:1:733:G:O2'	1:1:735:A:N6	2.38	0.46
4:4:182:ASP:HB3	4:4:236:CYS:SG	2.55	0.46
11:F:88:ARG:NH1	11:F:108:LEU:O	2.46	0.46
18:M:23:ILE:O	18:M:30:GLY:N	2.47	0.46
33:b:420:TYR:OH	33:b:428:LYS:CB	2.63	0.46
45:n:30:THR:O	45:n:34:LEU:HD13	2.15	0.46
51:t:338:ASP:O	51:t:338:ASP:OD2	2.33	0.46
51:t:487:ALA:O	51:t:491:ASP:OD2	2.34	0.46
54:y:118:HIS:CE1	54:y:146:ILE:HD12	2.51	0.46
1:1:2541:U:O2'	1:1:2542:U:OP2	2.27	0.46
4:4:43:THR:O	4:4:47:ASN:ND2	2.48	0.46
4:4:475:LEU:HD21	4:4:480:VAL:HG23	1.96	0.46
9:D:43:LYS:HB2	9:D:46:THR:HG21	1.97	0.46
35:d:11:GLU:O	35:d:106:THR:OG1	2.24	0.46
44:m:96:LEU:C	44:m:99:THR:HG22	2.40	0.46
44:m:96:LEU:O	44:m:99:THR:HG22	2.15	0.46
54:y:231:SER:O	54:y:234:GLY:N	2.46	0.46
1:1:1593:A:N3	1:1:1615:C:O2'	2.46	0.46
1:1:2392:C:O2'	7:B:266:ARG:NH2	2.48	0.46
17:L:131:LYS:H	17:L:131:LYS:HD3	1.80	0.46
21:P:25:SER:O	21:P:29:THR:HG22	2.15	0.46
3:3:35:C:O2	3:3:45:A:O2'	2.34	0.46
9:D:235:SER:HG	9:D:236:LEU:H	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:H:47:LYS:NZ	18:M:5:SER:O	2.39	0.46
18:M:40:ASP:OD1	18:M:43:LYS:N	2.47	0.46
19:N:190:THR:HG22	19:N:193:ARG:NH2	2.30	0.46
42:k:17:ARG:NE	42:k:19:ASP:OD1	2.46	0.46
1:1:2376:G:O2'	1:1:2377:G:O5'	2.23	0.46
1:1:2646:C:O2	1:1:2647:A:N6	2.48	0.46
4:4:79:TYR:OH	4:4:575:MET:SD	2.59	0.46
30:Y:59:VAL:HG22	30:Y:103:LYS:O	2.16	0.46
33:b:415:ASN:HB3	33:b:418:ASP:OD2	2.15	0.46
48:q:80:LEU:O	48:q:83:THR:OG1	2.30	0.46
51:t:213:ASP:OD2	51:t:214:GLN:NE2	2.49	0.46
4:4:142:THR:HB	4:4:155:SER:CB	2.46	0.46
5:5:43:SER:C	5:5:46:LEU:CD2	2.84	0.46
13:H:81:GLY:O	13:H:149:ASN:OD1	2.34	0.46
31:Z:33:SER:OG	31:Z:35:SER:O	2.28	0.46
49:r:185:THR:CB	49:r:192:THR:HG22	2.45	0.46
53:x:159:MET:SD	53:x:161:THR:HG23	2.56	0.46
4:4:270:THR:OG1	4:4:271:GLU:N	2.49	0.46
6:A:168:VAL:CG2	47:p:79:VAL:HG21	2.45	0.46
9:D:232:ASP:HB2	9:D:235:SER:OG	2.16	0.46
51:t:210:ASN:O	51:t:213:ASP:OD2	2.34	0.46
54:y:111:ASN:OD1	54:y:114:VAL:N	2.45	0.46
14:I:61:ALA:HB1	14:I:131:LEU:HD22	1.98	0.46
33:b:509:ASN:HD21	35:d:58:ALA:HB2	1.81	0.46
3:3:28:C:OP1	15:J:137:ARG:NH1	2.49	0.45
4:4:252:ALA:HB3	4:4:254:GLN:OE1	2.17	0.45
9:D:91:GLY:O	9:D:94:ASN:ND2	2.49	0.45
36:e:100:ILE:O	36:e:105:ARG:NH1	2.48	0.45
51:t:211:LEU:HD22	51:t:218:GLN:HB3	1.97	0.45
51:t:465:GLN:HA	51:t:468:VAL:HG22	1.97	0.45
53:x:157:SER:O	53:x:173:CYS:SG	2.71	0.45
6:A:143:GLU:O	6:A:144:ASN:C	2.58	0.45
9:D:261:THR:OG1	9:D:262:LYS:N	2.48	0.45
11:F:86:VAL:HG13	11:F:136:TYR:HB3	1.98	0.45
12:G:158:ASP:HB3	12:G:159:PRO:HD2	1.96	0.45
15:J:93:ASP:OD1	15:J:93:ASP:N	2.49	0.45
54:y:7:PHE:HZ	54:y:31:SER:HG	1.59	0.45
1:1:394:G:N1	1:1:397:A:OP2	2.44	0.45
1:1:1221:A:O2'	28:W:72:VAL:HG22	2.16	0.45
6:A:14:SER:OG	6:A:15:ILE:N	2.49	0.45
33:b:194:VAL:HG12	57:b:701:GTP:H5''	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:g:46:ASP:OD2	38:g:88:ARG:NH2	2.49	0.45
44:m:325:ASN:ND2	44:m:345:PRO:O	2.45	0.45
8:C:360:LYS:O	24:S:28:ARG:NH2	2.50	0.45
16:K:116:VAL:HA	16:K:119:ILE:HG22	1.97	0.45
31:Z:33:SER:OG	31:Z:34:LYS:N	2.49	0.45
31:Z:110:ALA:O	31:Z:114:VAL:HG23	2.17	0.45
1:1:1834:U:OP1	43:l:5:LYS:NZ	2.34	0.45
1:1:3002:C:O2'	7:B:180:GLU:OE2	2.28	0.45
1:1:3015:G:OP2	55:z:2:ALA:N	2.50	0.45
10:E:141:VAL:HG13	10:E:142:ASP:OD1	2.16	0.45
13:H:31:ARG:CD	13:H:149:ASN:OD1	2.64	0.45
16:K:67:ILE:HD11	16:K:105:SER:CB	2.47	0.45
22:Q:62:VAL:HB	22:Q:83:VAL:HG11	1.98	0.45
28:W:234:ASN:OD1	28:W:234:ASN:N	2.49	0.45
44:m:81:THR:OG1	49:r:222:GLU:OE1	2.24	0.45
51:t:187:LEU:HD23	51:t:187:LEU:O	2.16	0.45
21:P:120:ASN:OD1	21:P:145:HIS:HB2	2.16	0.45
29:X:10:ALA:O	29:X:14:VAL:HG23	2.17	0.45
33:b:177:ASN:OD1	33:b:197:TYR:C	2.59	0.45
53:x:160:VAL:HG11	53:x:201:ILE:HD13	1.97	0.45
23:R:102:LEU:HD22	23:R:138:LEU:HD22	1.99	0.45
30:Y:29:VAL:O	30:Y:32:SER:OG	2.35	0.45
33:b:232:MET:HE1	33:b:240:ILE:HD11	1.97	0.45
42:k:58:ASP:OD2	42:k:61:LYS:CB	2.65	0.45
51:t:187:LEU:HD23	51:t:187:LEU:C	2.41	0.45
51:t:385:ILE:HG23	51:t:386:TYR:CD2	2.52	0.45
53:x:446:SER:O	53:x:464:LYS:N	2.46	0.45
54:y:53:ILE:CG1	54:y:59:ILE:HG22	2.46	0.45
1:1:2473:C:O2'	1:1:2474:G:O4'	2.31	0.45
24:S:51:VAL:HG12	24:S:52:LYS:H	1.82	0.45
44:m:416:TYR:OH	44:m:462:ILE:HD11	2.17	0.45
48:q:82:ILE:HA	48:q:85:LEU:HD13	1.98	0.45
53:x:179:MET:HE3	53:x:180:HIS:CE1	2.52	0.45
1:1:269:G:OP2	19:N:44:ARG:NH2	2.43	0.45
4:4:466:LEU:O	4:4:467:THR:CG2	2.65	0.45
4:4:491:SER:O	4:4:492:THR:HB	2.17	0.45
25:T:152:ALA:HB1	25:T:153:PRO:HD2	1.97	0.45
27:V:54:LEU:O	27:V:54:LEU:HG	2.17	0.45
34:c:19:LYS:O	34:c:22:SER:HB3	2.17	0.45
1:1:1779:C:N4	23:R:88:ARG:O	2.49	0.44
7:B:163:HIS:ND1	7:B:164:THR:O	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:x:157:SER:C	53:x:173:CYS:SG	3.00	0.44
1:1:1300:G:OP1	49:r:44:GLY:N	2.50	0.44
4:4:453:ASN:N	4:4:453:ASN:OD1	2.49	0.44
8:C:156:LEU:HD12	8:C:159:ILE:HD12	1.98	0.44
17:L:153:ASP:OD2	17:L:154:VAL:N	2.48	0.44
32:a:76:ASP:OD1	32:a:77:LYS:N	2.49	0.44
33:b:536:SER:OG	52:u:143:ARG:NH2	2.50	0.44
1:1:912:G:N7	6:A:9:ARG:NH2	2.65	0.44
1:1:1523:U:OP1	1:1:1607:U:N3	2.46	0.44
1:1:2857:C:N4	1:1:2858:U:O4	2.50	0.44
4:4:179:GLY:O	4:4:182:ASP:HB2	2.18	0.44
4:4:231:ALA:HB1	4:4:236:CYS:O	2.18	0.44
8:C:140:HIS:O	8:C:142:VAL:HG13	2.18	0.44
28:W:38:ARG:N	28:W:106:ASP:OD1	2.49	0.44
1:1:215:G:OP1	30:Y:12:ARG:NH1	2.49	0.44
1:1:1249:G:OP1	44:m:144:LYS:NZ	2.46	0.44
1:1:3145:C:OP1	34:c:9:ARG:NH1	2.51	0.44
45:n:27:TYR:O	45:n:31:VAL:HG23	2.18	0.44
54:y:7:PHE:HZ	54:y:31:SER:OG	1.94	0.44
1:1:2625:C:O2'	1:1:2626:A:O5'	2.33	0.44
17:L:46:ILE:HG22	17:L:46:ILE:O	2.17	0.44
33:b:166:ASN:N	33:b:166:ASN:OD1	2.50	0.44
35:d:29:ALA:HB3	35:d:30:PRO:HD3	1.99	0.44
39:h:15:GLU:OE1	39:h:15:GLU:N	2.49	0.44
51:t:390:LEU:O	51:t:426:LYS:NZ	2.49	0.44
5:5:43:SER:HA	5:5:46:LEU:CD2	2.48	0.44
9:D:103:LEU:HD13	9:D:168:ASP:CB	2.47	0.44
49:r:189:LEU:O	49:r:191:VAL:HG23	2.17	0.44
1:1:3139:A:OP1	7:B:274:SER:OG	2.30	0.44
23:R:130:ASN:O	23:R:131:ALA:CB	2.65	0.44
24:S:11:GLY:N	24:S:41:TYR:OH	2.50	0.44
33:b:249:CYS:SG	33:b:250:VAL:N	2.90	0.44
46:o:101:LYS:O	46:o:104:SER:CB	2.66	0.44
9:D:67:SER:CB	9:D:72:ASP:CG	2.72	0.44
13:H:67:ALA:O	13:H:71:VAL:HG23	2.18	0.44
21:P:64:ASN:OD1	21:P:64:ASN:N	2.51	0.44
22:Q:64:VAL:HG23	22:Q:88:THR:O	2.18	0.44
1:1:297:G:OP2	1:1:297:G:N2	2.39	0.44
4:4:402:VAL:HG23	4:4:403:HIS:H	1.83	0.44
31:Z:75:VAL:HG11	31:Z:80:LEU:HD21	2.00	0.44
33:b:232:MET:HE1	33:b:240:ILE:CD1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:m:224:VAL:HG22	44:m:254:HIS:HD2	1.83	0.44
49:r:92:LEU:O	49:r:93:ASP:HB2	2.18	0.44
53:x:331:ASP:OD2	53:x:331:ASP:C	2.61	0.44
1:1:1012:G:O2'	1:1:1013:G:O5'	2.31	0.43
1:1:2600:C:OP1	19:N:93:LYS:NZ	2.50	0.43
1:1:2807:U:O2'	1:1:2809:C:OP1	2.33	0.43
1:1:2841:G:HO2'	1:1:2842:U:P	2.40	0.43
4:4:243:ARG:NH1	4:4:253:GLY:O	2.51	0.43
16:K:328:LEU:HD12	16:K:329:LEU:HG	2.00	0.43
22:Q:89:ASP:OD1	22:Q:90:ASP:N	2.49	0.43
1:1:388:G:N2	21:P:101:ASN:OD1	2.49	0.43
1:1:1935:G:OP1	44:m:441:GLY:N	2.51	0.43
12:G:84:ARG:NH2	29:X:14:VAL:O	2.51	0.43
13:H:103:ILE:HD11	13:H:134:ILE:HG22	2.00	0.43
14:I:58:MET:SD	14:I:58:MET:N	2.91	0.43
18:M:121:MET:HE3	18:M:125:LYS:NZ	2.34	0.43
25:T:54:HIS:CE1	25:T:89:LEU:CD1	2.98	0.43
25:T:80:VAL:HG23	25:T:85:LEU:HD21	1.99	0.43
27:V:36:ILE:CG1	27:V:60:ALA:CA	2.78	0.43
33:b:11:VAL:HG22	33:b:64:ILE:HD12	2.00	0.43
3:3:11:A:N6	9:D:13:SER:O	2.50	0.43
18:M:77:ARG:O	18:M:81:VAL:HG23	2.18	0.43
54:y:6:GLN:NE2	54:y:11:ASN:OD1	2.49	0.43
9:D:182:GLY:CA	9:D:194:LEU:HD23	2.48	0.43
16:K:51:ASN:OD1	16:K:51:ASN:N	2.50	0.43
33:b:420:TYR:CE2	33:b:428:LYS:NZ	2.86	0.43
51:t:334:HIS:C	51:t:335:LEU:HD12	2.43	0.43
53:x:296:SER:OG	53:x:297:HIS:N	2.51	0.43
3:3:39:C:O2'	15:J:44:THR:O	2.21	0.43
11:F:148:VAL:HG12	11:F:181:ILE:HD11	2.00	0.43
41:j:21:ARG:NH2	41:j:41:ALA:O	2.46	0.43
3:3:39:C:N3	15:J:70:THR:HG22	2.34	0.43
4:4:366:GLN:HG2	4:4:367:THR:N	2.34	0.43
7:B:155:ALA:O	7:B:157:VAL:N	2.43	0.43
31:Z:83:THR:HG22	31:Z:85:TYR:H	1.84	0.43
33:b:324:LEU:CD1	33:b:327:ASN:HB3	2.45	0.43
33:b:420:TYR:CE2	33:b:428:LYS:CD	2.85	0.43
53:x:449:GLN:C	53:x:462:CYS:HG	2.20	0.43
1:1:2249:G:H1	1:1:2268:U:H5	1.67	0.43
3:3:87:G:O2'	24:S:119:ARG:NH1	2.46	0.43
9:D:34:LYS:O	9:D:38:THR:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:D:104:LEU:HD11	9:D:108:ARG:NH2	2.34	0.43
15:J:172:LEU:O	15:J:173:ASP:CB	2.67	0.43
16:K:170:ARG:O	16:K:170:ARG:NH2	2.51	0.43
31:Z:27:LYS:HA	31:Z:28:PRO:HD2	1.83	0.43
33:b:86:TYR:O	33:b:149:TYR:OH	2.30	0.43
54:y:186:VAL:CG2	54:y:193:VAL:HG12	2.48	0.43
1:1:1241:U:HO2'	1:1:1242:G:P	2.39	0.43
3:3:11:A:O2'	3:3:13:A:OP2	2.29	0.43
4:4:329:CYS:O	4:4:331:LYS:N	2.52	0.43
8:C:358:THR:O	24:S:26:ARG:NE	2.52	0.43
11:F:130:ILE:O	11:F:134:VAL:HG22	2.19	0.43
27:V:19:VAL:HG13	27:V:37:ILE:HA	2.01	0.43
44:m:325:ASN:CG	57:m:501:GTP:H5'	2.44	0.43
1:1:713:U:OP1	17:L:174:ARG:NH2	2.52	0.43
4:4:475:LEU:CG	4:4:480:VAL:CG2	2.95	0.43
22:Q:44:PHE:CD1	22:Q:139:ILE:HD11	2.54	0.43
33:b:398:LEU:HD21	54:y:39:GLU:HB3	1.89	0.43
8:C:99:MET:HE1	8:C:103:THR:HG23	2.00	0.43
8:C:289:ILE:HG23	22:Q:129:VAL:CG1	2.49	0.43
33:b:172:ILE:HD13	33:b:183:PHE:CD2	2.54	0.43
54:y:7:PHE:HE1	54:y:31:SER:OG	1.99	0.43
9:D:65:ILE:HD12	9:D:74:VAL:HG22	1.99	0.42
9:D:232:ASP:N	9:D:232:ASP:OD2	2.52	0.42
11:F:173:LEU:HD23	11:F:176:TYR:HE2	1.84	0.42
1:1:2722:U:H4'	25:T:88:ARG:HG3	2.01	0.42
9:D:232:ASP:CB	9:D:235:SER:OG	2.68	0.42
24:S:155:ARG:H	24:S:170:THR:HG1	1.64	0.42
33:b:619:GLN:O	43:l:46:ARG:NH2	2.52	0.42
43:l:33:ASN:ND2	43:l:35:ILE:O	2.52	0.42
54:y:220:SER:OG	54:y:221:ILE:N	2.53	0.42
1:1:2338:C:H2'	1:1:2339:C:C6	2.54	0.42
1:1:3330:A:OP2	7:B:376:LYS:NZ	2.37	0.42
4:4:97:ILE:CG2	4:4:137:ASP:OD1	2.68	0.42
6:A:30:ARG:NH2	6:A:33:ASP:OD2	2.53	0.42
17:L:88:ALA:O	17:L:92:THR:HG23	2.19	0.42
24:S:77:VAL:HG12	24:S:126:VAL:HG13	2.00	0.42
27:V:104:ASN:OD1	27:V:108:GLU:N	2.51	0.42
1:1:42:C:O2'	1:1:2802:A:N6	2.53	0.42
1:1:348:A:N3	1:1:352:A:O2'	2.51	0.42
1:1:1646:G:O2'	1:1:1808:G:N2	2.44	0.42
1:1:2632:G:N1	1:1:2647:A:N7	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:M:15:VAL:HG22	18:M:65:LEU:HD11	2.00	0.42
19:N:103:GLU:OE1	19:N:118:SER:OG	2.23	0.42
21:P:127:ARG:NH2	21:P:139:TYR:HD2	2.15	0.42
33:b:278:PHE:HB3	33:b:283:VAL:HG21	2.00	0.42
33:b:547:ASP:OD1	33:b:547:ASP:N	2.52	0.42
48:q:64:ILE:HD12	48:q:68:GLN:O	2.18	0.42
4:4:546:GLN:O	4:4:547:ASP:OD1	2.38	0.42
7:B:221:THR:HG21	7:B:275:ARG:HG3	2.02	0.42
18:M:55:ARG:NH2	18:M:76:ALA:O	2.51	0.42
1:1:1724:U:O2'	1:1:1725:C:OP2	2.28	0.42
4:4:105:CYS:SG	4:4:391:LYS:NZ	2.93	0.42
4:4:221:GLN:OE1	4:4:221:GLN:N	2.53	0.42
8:C:260:GLN:N	8:C:260:GLN:OE1	2.52	0.42
15:J:141:ARG:HE	15:J:144:CYS:HB3	1.84	0.42
33:b:343:ARG:NH1	54:y:242:GLU:OE2	2.53	0.42
33:b:544:ALA:C	33:b:547:ASP:OD1	2.62	0.42
48:q:42:VAL:HG12	48:q:69:ALA:CB	2.49	0.42
48:q:143:VAL:CG1	48:q:151:ILE:HD12	2.49	0.42
51:t:47:MET:SD	51:t:119:HIS:NE2	2.90	0.42
1:1:2669:G:OP1	5:5:108:ARG:NH1	2.51	0.42
11:F:189:ILE:HG23	11:F:190:THR:HG23	2.01	0.42
15:J:90:GLN:HG3	15:J:170:ASP:OD1	2.20	0.42
19:N:13:LYS:O	19:N:19:LEU:HD22	2.19	0.42
19:N:97:SER:OG	19:N:167:THR:OG1	2.29	0.42
25:T:103:GLN:HE21	25:T:104:GLU:H	1.68	0.42
37:f:49:ILE:HD11	37:f:71:VAL:CG2	2.50	0.42
51:t:43:ARG:NE	51:t:111:GLU:OE1	2.51	0.42
54:y:122:ASP:OD1	54:y:123:ARG:N	2.53	0.42
1:1:971:G:P	22:Q:8:LYS:HZ3	2.37	0.42
1:1:2393:G:O2'	1:1:2982:A:N6	2.53	0.42
21:P:6:ALA:HB1	34:c:85:THR:O	2.19	0.42
24:S:109:ASP:OD1	24:S:113:ARG:NH1	2.53	0.42
29:X:34:LEU:HD23	29:X:35:PRO:O	2.20	0.42
51:t:385:ILE:CG2	51:t:386:TYR:N	2.82	0.42
1:1:1747:G:H21	42:k:2:ALA:HB3	1.85	0.42
13:H:31:ARG:CG	13:H:149:ASN:OD1	2.67	0.42
25:T:71:SER:O	25:T:72:VAL:HG13	2.20	0.42
33:b:194:VAL:HG13	57:b:701:GTP:O2A	2.19	0.42
33:b:318:MET:HE1	33:b:330:GLU:CD	2.44	0.42
47:p:56:THR:HB	47:p:63:THR:HG23	2.02	0.42
54:y:21:ASN:O	54:y:202:TYR:OH	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:164:ASP:OD1	4:4:173:THR:CA	2.68	0.42
9:D:103:LEU:HD13	9:D:168:ASP:HB3	2.00	0.42
13:H:21:LYS:CG	13:H:22:SER:N	2.82	0.42
14:I:125:GLU:C	14:I:125:GLU:OE2	2.63	0.42
25:T:54:HIS:O	25:T:55:LYS:C	2.63	0.42
27:V:89:ASP:O	27:V:89:ASP:OD2	2.38	0.42
52:u:80:ARG:NH2	54:y:88:LEU:O	2.48	0.42
4:4:466:LEU:O	4:4:467:THR:HG23	2.19	0.41
4:4:539:SER:OG	4:4:540:GLN:N	2.53	0.41
7:B:103:THR:HG23	7:B:151:ILE:HD11	2.02	0.41
9:D:239:ILE:O	9:D:242:SER:CB	2.61	0.41
10:E:100:LYS:NZ	10:E:137:ASP:OD2	2.43	0.41
27:V:18:PRO:HA	27:V:51:ALA:HB2	2.01	0.41
1:1:2411:U:HO2'	1:1:2412:G:C5'	2.33	0.41
1:1:3165:A:H62	1:1:3285:C:N4	2.18	0.41
1:1:3272:C:OP2	10:E:78:ARG:NH2	2.50	0.41
4:4:487:SER:O	4:4:491:SER:HB3	2.21	0.41
7:B:212:ASN:OD1	7:B:354:VAL:HG12	2.19	0.41
27:V:38:ALA:HB3	27:V:59:MET:HB2	2.00	0.41
54:y:28:VAL:HG12	54:y:52:THR:HG23	2.02	0.41
54:y:154:LEU:CD1	54:y:177:LEU:HD13	2.51	0.41
4:4:218:ILE:O	4:4:310:VAL:HG22	2.20	0.41
12:G:162:LEU:HA	19:N:7:LEU:HD11	2.02	0.41
14:I:35:LEU:HD21	14:I:123:LEU:HD21	2.02	0.41
24:S:57:GLU:OE2	25:T:139:ARG:NH2	2.53	0.41
31:Z:76:ASN:OD1	31:Z:77:TYR:N	2.53	0.41
31:Z:95:VAL:HG13	31:Z:96:VAL:N	2.35	0.41
42:k:32:ASN:OD1	42:k:33:LYS:NZ	2.34	0.41
44:m:418:ILE:CD1	44:m:421:TRP:CZ3	3.01	0.41
53:x:453:SER:OG	53:x:455:ASP:OD1	2.11	0.41
2:2:74:U:O4	30:Y:72:SER:OG	2.37	0.41
4:4:264:TYR:HE2	4:4:304:ILE:CD1	2.33	0.41
7:B:35:ASP:OD2	7:B:191:LYS:NZ	2.54	0.41
30:Y:109:LEU:HD22	30:Y:115:ARG:NH1	2.35	0.41
33:b:59:GLU:O	33:b:63:ASP:OD2	2.37	0.41
44:m:245:TYR:O	44:m:249:GLU:HB2	2.20	0.41
51:t:187:LEU:C	51:t:187:LEU:CD2	2.93	0.41
53:x:447:VAL:HG13	53:x:462:CYS:O	2.20	0.41
1:1:2898:G:H22	49:r:7:ILE:H	1.69	0.41
10:E:31:ARG:NH2	10:E:81:ALA:O	2.51	0.41
19:N:153:ASP:N	19:N:153:ASP:OD2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:b:446:ASP:OD1	33:b:446:ASP:N	2.53	0.41
45:n:98:SER:OG	45:n:99:ASP:N	2.53	0.41
51:t:222:ALA:O	51:t:226:THR:HG23	2.20	0.41
5:5:73:GLN:O	5:5:77:THR:HG23	2.19	0.41
9:D:223:PHE:O	9:D:227:LEU:N	2.49	0.41
44:m:228:VAL:HG21	44:m:328:LYS:HG2	2.01	0.41
54:y:187:ASN:OD1	54:y:210:THR:HB	2.21	0.41
1:1:1613:A:OP1	42:k:2:ALA:N	2.53	0.41
7:B:281:LYS:NZ	7:B:349:LYS:O	2.51	0.41
11:F:82:LYS:C	11:F:119:VAL:HG12	2.46	0.41
13:H:76:ASP:O	13:H:80:THR:HG23	2.21	0.41
33:b:569:ASP:OD1	33:b:570:GLN:N	2.54	0.41
35:d:47:ASP:OD1	35:d:47:ASP:N	2.54	0.41
44:m:99:THR:HG23	44:m:100:GLN:N	2.36	0.41
44:m:214:GLU:O	44:m:218:VAL:HG23	2.20	0.41
44:m:330:SER:OG	57:m:501:GTP:O2A	2.37	0.41
51:t:385:ILE:CG2	51:t:386:TYR:CE2	3.04	0.41
1:1:309:U:OP1	40:i:84:LYS:NZ	2.48	0.41
1:1:2651:G:O2'	1:1:2652:U:O5'	2.31	0.41
23:R:135:LYS:O	23:R:139:VAL:HG23	2.20	0.41
33:b:226:ASP:O	33:b:227:ARG:C	2.62	0.41
33:b:227:ARG:O	33:b:229:THR:N	2.54	0.41
48:q:136:ALA:HB1	48:q:141:CYS:SG	2.61	0.41
49:r:155:THR:HG22	49:r:156:PHE:N	2.36	0.41
53:x:348:THR:HG23	53:x:351:GLU:H	1.84	0.41
53:x:377:ALA:HB2	53:x:408:VAL:CG2	2.51	0.41
54:y:186:VAL:O	54:y:190:SER:N	2.53	0.41
1:1:831:G:O2'	1:1:1864:A:N3	2.47	0.41
1:1:1039:U:OP1	5:5:112:LYS:NZ	2.50	0.41
1:1:1277:C:O2'	1:1:1278:A:O4'	2.38	0.41
1:1:1813:A:O2'	1:1:1816:A:N3	2.54	0.41
1:1:2473:C:H6	1:1:2474:G:H21	1.68	0.41
1:1:3163:A:N6	1:1:3287:U:O2'	2.54	0.41
4:4:218:ILE:O	4:4:310:VAL:HG13	2.20	0.41
4:4:250:PHE:C	4:4:251:LEU:HD12	2.46	0.41
9:D:68:THR:HG22	9:D:69:ILE:H	1.86	0.41
17:L:109:PHE:O	17:L:113:VAL:HG23	2.20	0.41
21:P:29:THR:HA	21:P:32:THR:HG22	2.03	0.41
32:a:114:GLY:O	32:a:137:LYS:NZ	2.47	0.41
33:b:422:LEU:HD13	33:b:427:TRP:NE1	2.35	0.41
44:m:75:ARG:HG2	44:m:75:ARG:HH11	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:o:37:GLY:O	46:o:203:SER:N	2.53	0.41
51:t:166:SER:O	51:t:166:SER:OG	2.38	0.41
1:1:1483:G:O6	38:g:4:ARG:NH2	2.48	0.41
1:1:1643:A:O2'	1:1:1644:C:O4'	2.34	0.41
1:1:2276:G:OP2	1:1:2316:G:N2	2.51	0.41
1:1:3217:C:O2'	1:1:3217:C:O2	2.32	0.41
2:2:39:G:O2'	2:2:105:A:N1	2.51	0.41
4:4:467:THR:CG2	33:b:575:ALA:H	2.28	0.41
8:C:140:HIS:O	8:C:142:VAL:N	2.54	0.41
14:I:54:CYS:O	14:I:56:LYS:N	2.54	0.41
16:K:186:TRP:CE2	16:K:303:ILE:HG21	2.56	0.41
19:N:110:ALA:HB1	19:N:113:LEU:CD2	2.41	0.41
32:a:77:LYS:O	32:a:79:TRP:N	2.54	0.41
51:t:91:VAL:O	51:t:95:SER:OG	2.30	0.41
54:y:59:ILE:O	54:y:63:THR:OG1	2.29	0.41
1:1:1940:G:H21	1:1:3362:A:H8	1.69	0.40
4:4:94:THR:HB	4:4:142:THR:CG2	2.51	0.40
6:A:7:ASN:OD1	6:A:8:GLN:N	2.54	0.40
6:A:79:ASN:ND2	6:A:166:ILE:O	2.51	0.40
17:L:107:GLU:OE1	17:L:107:GLU:N	2.50	0.40
24:S:27:MET:HE1	24:S:44:PHE:CB	2.51	0.40
25:T:54:HIS:HD2	25:T:57:TYR:CE2	2.37	0.40
33:b:185:ARG:NH1	33:b:192:VAL:O	2.54	0.40
33:b:280:ASN:OD1	33:b:280:ASN:N	2.55	0.40
33:b:324:LEU:HD11	33:b:327:ASN:HB2	1.97	0.40
38:g:101:VAL:HA	38:g:104:VAL:HG22	2.03	0.40
39:h:79:ASP:OD2	39:h:79:ASP:N	2.54	0.40
1:1:1517:G:O2'	33:b:579:ASN:ND2	2.50	0.40
1:1:2272:G:H22	16:K:60:THR:HB	1.85	0.40
28:W:45:LEU:HB3	28:W:48:VAL:HG21	2.03	0.40
33:b:595:ASP:OD2	33:b:597:SER:OG	2.35	0.40
36:e:98:HIS:O	36:e:125:ARG:NH2	2.54	0.40
53:x:449:GLN:HG2	53:x:462:CYS:SG	2.60	0.40
1:1:1846:C:O2	33:b:625:HIS:NE2	2.47	0.40
16:K:54:ASP:OD2	16:K:55:LEU:HD13	2.22	0.40
1:1:3187:A:OP1	13:H:23:ARG:NE	2.54	0.40
1:1:3215:A:C5'	18:M:121:MET:HE1	2.49	0.40
4:4:244:VAL:HG23	4:4:319:ILE:HD13	2.02	0.40
9:D:68:THR:HB	9:D:70:THR:HG22	2.04	0.40
10:E:30:LEU:HD11	10:E:57:HIS:ND1	2.35	0.40
16:K:54:ASP:OD2	16:K:55:LEU:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:S:9:VAL:HG22	24:S:61:ILE:HD12	2.02	0.40
1:1:610:G:C8	8:C:312:VAL:HG21	2.57	0.40
1:1:839:C:O2'	1:1:1724:U:OP1	2.39	0.40
48:q:42:VAL:HG12	48:q:69:ALA:HB2	2.04	0.40
53:x:157:SER:C	53:x:173:CYS:HG	2.25	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	4	495/593 (84%)	456 (92%)	34 (7%)	5 (1%)	12	45
5	5	76/120 (63%)	71 (93%)	5 (7%)	0	100	100
6	A	243/254 (96%)	227 (93%)	16 (7%)	0	100	100
7	B	384/387 (99%)	342 (89%)	41 (11%)	1 (0%)	36	70
8	C	359/362 (99%)	336 (94%)	21 (6%)	2 (1%)	21	56
9	D	239/297 (80%)	218 (91%)	21 (9%)	0	100	100
10	E	152/176 (86%)	148 (97%)	4 (3%)	0	100	100
11	F	214/244 (88%)	195 (91%)	19 (9%)	0	100	100
12	G	226/256 (88%)	209 (92%)	17 (8%)	0	100	100
13	H	185/191 (97%)	172 (93%)	13 (7%)	0	100	100
14	I	128/166 (77%)	113 (88%)	13 (10%)	2 (2%)	7	34
15	J	166/174 (95%)	145 (87%)	20 (12%)	1 (1%)	21	56
16	K	226/334 (68%)	210 (93%)	14 (6%)	2 (1%)	14	48
17	L	179/199 (90%)	165 (92%)	12 (7%)	2 (1%)	11	43
18	M	132/138 (96%)	126 (96%)	6 (4%)	0	100	100
19	N	201/204 (98%)	187 (93%)	14 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	O	195/199 (98%)	194 (100%)	1 (0%)	0	100	100
21	P	167/184 (91%)	155 (93%)	12 (7%)	0	100	100
22	Q	142/186 (76%)	131 (92%)	11 (8%)	0	100	100
23	R	149/189 (79%)	142 (95%)	7 (5%)	0	100	100
24	S	169/172 (98%)	156 (92%)	10 (6%)	3 (2%)	6	31
25	T	120/160 (75%)	115 (96%)	5 (4%)	0	100	100
26	U	99/121 (82%)	95 (96%)	4 (4%)	0	100	100
27	V	132/137 (96%)	120 (91%)	10 (8%)	2 (2%)	8	35
28	W	231/236 (98%)	225 (97%)	4 (2%)	2 (1%)	14	48
29	X	138/142 (97%)	130 (94%)	8 (6%)	0	100	100
30	Y	123/127 (97%)	119 (97%)	4 (3%)	0	100	100
31	Z	133/136 (98%)	118 (89%)	15 (11%)	0	100	100
32	a	91/149 (61%)	84 (92%)	5 (6%)	2 (2%)	5	26
33	b	600/647 (93%)	538 (90%)	58 (10%)	4 (1%)	18	53
34	c	103/175 (59%)	99 (96%)	4 (4%)	0	100	100
35	d	103/113 (91%)	100 (97%)	3 (3%)	0	100	100
36	e	125/130 (96%)	122 (98%)	3 (2%)	0	100	100
37	f	104/107 (97%)	103 (99%)	1 (1%)	0	100	100
38	g	105/121 (87%)	104 (99%)	1 (1%)	0	100	100
39	h	117/120 (98%)	113 (97%)	4 (3%)	0	100	100
40	i	94/100 (94%)	85 (90%)	8 (8%)	1 (1%)	11	43
41	j	82/88 (93%)	80 (98%)	2 (2%)	0	100	100
42	k	75/78 (96%)	71 (95%)	4 (5%)	0	100	100
43	l	47/51 (92%)	44 (94%)	3 (6%)	0	100	100
44	m	431/486 (89%)	390 (90%)	38 (9%)	3 (1%)	18	53
45	n	95/105 (90%)	92 (97%)	3 (3%)	0	100	100
46	o	167/217 (77%)	145 (87%)	22 (13%)	0	100	100
47	p	87/92 (95%)	84 (97%)	2 (2%)	1 (1%)	11	43
48	q	120/165 (73%)	101 (84%)	16 (13%)	3 (2%)	4	23
49	r	219/261 (84%)	197 (90%)	20 (9%)	2 (1%)	14	48
50	s	52/520 (10%)	47 (90%)	3 (6%)	2 (4%)	2	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	t	425/767 (55%)	399 (94%)	26 (6%)	0	100	100
52	u	146/199 (73%)	139 (95%)	7 (5%)	0	100	100
53	x	386/515 (75%)	364 (94%)	22 (6%)	0	100	100
54	y	241/245 (98%)	220 (91%)	20 (8%)	1 (0%)	30	65
55	z	73/106 (69%)	67 (92%)	6 (8%)	0	100	100
All	All	9491/11641 (82%)	8808 (93%)	642 (7%)	41 (0%)	31	65

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	C	339	LEU
28	W	177	ALA
33	b	398	LEU
33	b	399	ALA
4	4	329	CYS
4	4	363	ASP
7	B	386	ASP
17	L	63	VAL
17	L	165	SER
27	V	54	LEU
32	a	78	LEU
44	m	419	SER
49	r	17	ARG
50	s	12	SER
4	4	463	THR
4	4	467	THR
14	I	18	LEU
15	J	165	GLN
24	S	13	ARG
24	S	18	SER
24	S	85	SER
28	W	178	GLY
47	p	60	CYS
50	s	13	THR
14	I	17	ASP
32	a	77	LYS
33	b	576	SER
8	C	268	ALA
16	K	25	LYS
16	K	28	ALA

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Mol	Chain	Res	Type
48	q	120	SER
48	q	144	ASP
4	4	544	ASN
40	i	18	THR
44	m	157	LEU
48	q	17	ALA
49	r	206	SER
44	m	418	ILE
27	V	36	ILE
33	b	228	PRO
54	y	135	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	4	445/520 (86%)	445 (100%)	0	100	100
5	5	70/106 (66%)	70 (100%)	0	100	100
6	A	188/196 (96%)	188 (100%)	0	100	100
7	B	322/323 (100%)	321 (100%)	1 (0%)	86	91
8	C	288/289 (100%)	288 (100%)	0	100	100
9	D	205/245 (84%)	205 (100%)	0	100	100
10	E	134/153 (88%)	134 (100%)	0	100	100
11	F	183/205 (89%)	183 (100%)	0	100	100
12	G	187/208 (90%)	187 (100%)	0	100	100
13	H	167/171 (98%)	167 (100%)	0	100	100
14	I	116/141 (82%)	116 (100%)	0	100	100
15	J	146/150 (97%)	146 (100%)	0	100	100
16	K	214/302 (71%)	214 (100%)	0	100	100
17	L	145/159 (91%)	145 (100%)	0	100	100
18	M	107/109 (98%)	106 (99%)	1 (1%)	70	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	N	175/176 (99%)	175 (100%)	0	100	100
20	O	160/162 (99%)	160 (100%)	0	100	100
21	P	139/146 (95%)	139 (100%)	0	100	100
22	Q	118/151 (78%)	118 (100%)	0	100	100
23	R	125/154 (81%)	125 (100%)	0	100	100
24	S	155/156 (99%)	155 (100%)	0	100	100
25	T	107/137 (78%)	106 (99%)	1 (1%)	70	85
26	U	88/107 (82%)	87 (99%)	1 (1%)	65	83
27	V	103/105 (98%)	101 (98%)	2 (2%)	50	76
28	W	210/213 (99%)	210 (100%)	0	100	100
29	X	116/118 (98%)	116 (100%)	0	100	100
30	Y	108/110 (98%)	108 (100%)	0	100	100
31	Z	115/116 (99%)	115 (100%)	0	100	100
32	a	76/119 (64%)	76 (100%)	0	100	100
33	b	541/573 (94%)	539 (100%)	2 (0%)	84	90
34	c	99/153 (65%)	99 (100%)	0	100	100
35	d	92/97 (95%)	92 (100%)	0	100	100
36	e	109/111 (98%)	109 (100%)	0	100	100
37	f	90/91 (99%)	90 (100%)	0	100	100
38	g	92/103 (89%)	92 (100%)	0	100	100
39	h	104/105 (99%)	104 (100%)	0	100	100
40	i	78/82 (95%)	78 (100%)	0	100	100
41	j	69/71 (97%)	69 (100%)	0	100	100
42	k	68/69 (99%)	68 (100%)	0	100	100
43	l	44/46 (96%)	44 (100%)	0	100	100
44	m	388/428 (91%)	385 (99%)	3 (1%)	73	86
45	n	81/88 (92%)	81 (100%)	0	100	100
47	p	70/72 (97%)	70 (100%)	0	100	100
48	q	105/136 (77%)	105 (100%)	0	100	100
49	r	198/229 (86%)	197 (100%)	1 (0%)	81	89
50	s	50/445 (11%)	50 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
51	t	379/665 (57%)	379 (100%)	0	100	100
52	u	131/180 (73%)	130 (99%)	1 (1%)	73	86
53	x	338/451 (75%)	338 (100%)	0	100	100
54	y	209/211 (99%)	209 (100%)	0	100	100
55	z	69/95 (73%)	69 (100%)	0	100	100
All	All	8116/9748 (83%)	8103 (100%)	13 (0%)	85	92

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	B	84	VAL
18	M	64	VAL
25	T	128	LEU
26	U	52	ASN
27	V	36	ILE
27	V	85	TRP
33	b	420	TYR
33	b	440	ASN
44	m	28	ASN
44	m	82	ARG
44	m	83	VAL
49	r	168	MET
52	u	19	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
4	4	255	ASN
4	4	274	GLN
7	B	68	HIS
7	B	165	GLN
7	B	224	HIS
8	C	48	GLN
8	C	116	ASN
8	C	196	ASN
8	C	304	GLN
8	C	322	GLN
10	E	97	ASN
11	F	37	ASN

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Mol	Chain	Res	Type
11	F	186	HIS
11	F	194	HIS
12	G	24	ASN
12	G	61	GLN
12	G	77	GLN
12	G	232	HIS
13	H	49	ASN
13	H	58	HIS
13	H	59	ASN
13	H	96	HIS
15	J	47	GLN
15	J	90	GLN
16	K	12	GLN
17	L	12	ASN
17	L	120	GLN
17	L	149	GLN
18	M	41	GLN
19	N	195	ASN
20	O	55	HIS
22	Q	126	GLN
23	R	141	HIS
24	S	8	GLN
25	T	103	GLN
25	T	131	GLN
27	V	132	ASN
30	Y	42	GLN
33	b	208	HIS
33	b	217	GLN
33	b	367	GLN
33	b	384	ASN
33	b	415	ASN
33	b	498	ASN
33	b	509	ASN
33	b	619	GLN
34	c	44	ASN
34	c	61	ASN
34	c	64	ASN
40	i	12	ASN
42	k	10	GLN
44	m	310	HIS
44	m	408	GLN
44	m	411	HIS

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Mol	Chain	Res	Type
47	p	25	GLN
48	q	103	ASN
48	q	149	HIS
51	t	29	GLN
52	u	7	HIS
52	u	24	ASN
52	u	101	GLN
53	x	176	GLN
53	x	307	ASN
53	x	424	ASN
55	z	31	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3013/3396 (88%)	603 (20%)	26 (0%)
2	2	152/158 (96%)	27 (17%)	1 (0%)
3	3	115/121 (95%)	19 (16%)	1 (0%)
All	All	3280/3675 (89%)	649 (19%)	28 (0%)

All (649) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	13	A
1	1	14	U
1	1	18	G
1	1	26	A
1	1	30	G
1	1	40	A
1	1	41	G
1	1	43	A
1	1	49	A
1	1	57	A
1	1	59	G
1	1	60	A
1	1	65	A
1	1	66	A
1	1	73	C
1	1	76	G
1	1	92	G
1	1	94	G

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Mol	Chain	Res	Type
1	1	110	G
1	1	111	C
1	1	121	A
1	1	122	A
1	1	133	U
1	1	136	G
1	1	156	G
1	1	157	A
1	1	161	G
1	1	164	A
1	1	166	C
1	1	173	G
1	1	176	G
1	1	177	U
1	1	190	U
1	1	191	U
1	1	200	C
1	1	210	U
1	1	211	A
1	1	218	G
1	1	219	A
1	1	220	G
1	1	240	U
1	1	242	C
1	1	243	G
1	1	244	G
1	1	245	U
1	1	246	U
1	1	249	U
1	1	250	U
1	1	251	G
1	1	252	U
1	1	253	A
1	1	254	A
1	1	269	G
1	1	284	A
1	1	286	U
1	1	295	A
1	1	298	U
1	1	305	U
1	1	306	A
1	1	307	A

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Mol	Chain	Res	Type
1	1	329	U
1	1	338	A
1	1	339	C
1	1	346	C
1	1	352	A
1	1	362	U
1	1	376	G
1	1	386	A
1	1	398	A
1	1	399	A
1	1	401	U
1	1	402	A
1	1	403	C
1	1	421	G
1	1	422	A
1	1	516	A
1	1	521	A
1	1	523	A
1	1	525	C
1	1	536	U
1	1	543	C
1	1	545	U
1	1	547	G
1	1	552	G
1	1	555	U
1	1	557	A
1	1	559	A
1	1	569	A
1	1	578	A
1	1	579	G
1	1	597	G
1	1	604	G
1	1	607	A
1	1	609	G
1	1	610	G
1	1	611	A
1	1	620	U
1	1	621	A
1	1	622	A
1	1	637	C
1	1	643	U
1	1	644	G

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Mol	Chain	Res	Type
1	1	645	A
1	1	646	A
1	1	650	C
1	1	667	C
1	1	677	A
1	1	681	U
1	1	683	U
1	1	691	A
1	1	705	A
1	1	709	A
1	1	715	A
1	1	719	U
1	1	720	A
1	1	721	G
1	1	722	G
1	1	735	A
1	1	763	G
1	1	765	C
1	1	767	U
1	1	780	A
1	1	781	G
1	1	784	A
1	1	785	G
1	1	801	A
1	1	806	A
1	1	808	A
1	1	817	A
1	1	830	A
1	1	845	G
1	1	848	A
1	1	849	C
1	1	861	C
1	1	874	U
1	1	875	G
1	1	896	A
1	1	907	G
1	1	908	G
1	1	914	A
1	1	916	G
1	1	917	A
1	1	925	A
1	1	944	C

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Mol	Chain	Res	Type
1	1	953	G
1	1	955	U
1	1	956	U
1	1	958	C
1	1	961	C
1	1	962	A
1	1	964	G
1	1	966	U
1	1	976	U
1	1	977	C
1	1	978	G
1	1	979	U
1	1	980	A
1	1	981	U
1	1	984	G
1	1	991	G
1	1	1007	U
1	1	1008	U
1	1	1010	G
1	1	1013	G
1	1	1016	C
1	1	1017	C
1	1	1018	G
1	1	1019	G
1	1	1025	A
1	1	1026	A
1	1	1027	A
1	1	1028	U
1	1	1029	G
1	1	1030	A
1	1	1032	C
1	1	1034	U
1	1	1035	G
1	1	1036	A
1	1	1037	C
1	1	1038	C
1	1	1040	A
1	1	1044	U
1	1	1064	A
1	1	1066	G
1	1	1068	C
1	1	1072	G

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Mol	Chain	Res	Type
1	1	1073	U
1	1	1074	U
1	1	1084	A
1	1	1090	G
1	1	1098	A
1	1	1099	A
1	1	1112	A
1	1	1116	G
1	1	1117	G
1	1	1118	C
1	1	1123	U
1	1	1127	G
1	1	1128	U
1	1	1129	A
1	1	1131	G
1	1	1132	C
1	1	1135	A
1	1	1143	A
1	1	1153	A
1	1	1159	A
1	1	1161	G
1	1	1180	A
1	1	1181	U
1	1	1182	A
1	1	1186	G
1	1	1192	C
1	1	1193	A
1	1	1196	C
1	1	1198	C
1	1	1199	C
1	1	1200	A
1	1	1203	A
1	1	1209	G
1	1	1218	U
1	1	1222	G
1	1	1227	C
1	1	1240	A
1	1	1245	A
1	1	1254	C
1	1	1258	U
1	1	1262	G
1	1	1263	A

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Mol	Chain	Res	Type
1	1	1271	A
1	1	1272	C
1	1	1278	A
1	1	1287	A
1	1	1292	C
1	1	1302	A
1	1	1303	A
1	1	1304	A
1	1	1305	U
1	1	1307	G
1	1	1308	A
1	1	1309	U
1	1	1313	G
1	1	1330	A
1	1	1345	G
1	1	1348	U
1	1	1356	U
1	1	1386	A
1	1	1392	G
1	1	1399	A
1	1	1400	G
1	1	1405	U
1	1	1419	A
1	1	1434	G
1	1	1436	U
1	1	1437	C
1	1	1443	G
1	1	1455	U
1	1	1483	G
1	1	1484	U
1	1	1487	G
1	1	1503	A
1	1	1508	C
1	1	1522	U
1	1	1523	U
1	1	1533	U
1	1	1536	G
1	1	1539	A
1	1	1555	U
1	1	1556	C
1	1	1557	A
1	1	1560	G

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Mol	Chain	Res	Type
1	1	1561	G
1	1	1562	C
1	1	1575	A
1	1	1581	C
1	1	1582	C
1	1	1583	A
1	1	1588	A
1	1	1589	A
1	1	1629	U
1	1	1630	U
1	1	1639	C
1	1	1642	A
1	1	1643	A
1	1	1644	C
1	1	1657	C
1	1	1683	A
1	1	1717	U
1	1	1724	U
1	1	1725	C
1	1	1742	U
1	1	1750	A
1	1	1751	G
1	1	1760	A
1	1	1762	C
1	1	1763	U
1	1	1765	U
1	1	1766	G
1	1	1775	G
1	1	1780	G
1	1	1794	G
1	1	1797	A
1	1	1810	A
1	1	1813	A
1	1	1814	A
1	1	1815	U
1	1	1816	A
1	1	1821	U
1	1	1839	A
1	1	1842	A
1	1	1849	C
1	1	1850	A
1	1	1851	G

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Mol	Chain	Res	Type
1	1	1878	G
1	1	1880	U
1	1	1889	G
1	1	1901	A
1	1	1906	G
1	1	1925	U
1	1	1926	C
1	1	1951	C
1	1	1953	G
1	1	2102	U
1	1	2112	U
1	1	2121	G
1	1	2122	G
1	1	2126	A
1	1	2131	A
1	1	2134	G
1	1	2149	A
1	1	2169	G
1	1	2170	U
1	1	2184	U
1	1	2194	G
1	1	2205	U
1	1	2239	G
1	1	2244	A
1	1	2246	G
1	1	2248	C
1	1	2249	G
1	1	2267	C
1	1	2268	U
1	1	2270	A
1	1	2271	A
1	1	2272	G
1	1	2273	G
1	1	2276	G
1	1	2319	U
1	1	2320	A
1	1	2334	U
1	1	2335	G
1	1	2336	U
1	1	2338	C
1	1	2339	C
1	1	2340	U

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Mol	Chain	Res	Type
1	1	2373	A
1	1	2376	G
1	1	2377	G
1	1	2388	U
1	1	2391	G
1	1	2394	G
1	1	2397	A
1	1	2398	A
1	1	2399	A
1	1	2410	U
1	1	2411	U
1	1	2412	G
1	1	2418	G
1	1	2419	A
1	1	2435	G
1	1	2437	G
1	1	2444	C
1	1	2445	A
1	1	2448	G
1	1	2450	G
1	1	2452	G
1	1	2453	U
1	1	2459	A
1	1	2462	A
1	1	2463	G
1	1	2467	G
1	1	2468	A
1	1	2469	G
1	1	2470	C
1	1	2472	U
1	1	2473	C
1	1	2474	G
1	1	2476	C
1	1	2477	G
1	1	2480	A
1	1	2487	U
1	1	2493	U
1	1	2494	A
1	1	2502	A
1	1	2505	U
1	1	2514	U
1	1	2515	A

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Mol	Chain	Res	Type
1	1	2522	G
1	1	2524	A
1	1	2530	G
1	1	2531	C
1	1	2532	U
1	1	2534	G
1	1	2537	U
1	1	2538	U
1	1	2539	C
1	1	2540	A
1	1	2541	U
1	1	2542	U
1	1	2543	U
1	1	2546	C
1	1	2547	A
1	1	2548	C
1	1	2549	G
1	1	2552	C
1	1	2554	A
1	1	2561	A
1	1	2569	A
1	1	2570	U
1	1	2571	U
1	1	2572	C
1	1	2573	G
1	1	2586	G
1	1	2593	A
1	1	2595	A
1	1	2606	G
1	1	2607	G
1	1	2626	A
1	1	2629	U
1	1	2630	C
1	1	2631	U
1	1	2633	U
1	1	2634	U
1	1	2646	C
1	1	2647	A
1	1	2651	G
1	1	2652	U
1	1	2655	U
1	1	2656	A

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Mol	Chain	Res	Type
1	1	2657	A
1	1	2660	G
1	1	2661	G
1	1	2674	A
1	1	2677	G
1	1	2681	U
1	1	2689	A
1	1	2694	A
1	1	2697	A
1	1	2698	G
1	1	2704	A
1	1	2714	G
1	1	2720	G
1	1	2730	G
1	1	2732	G
1	1	2736	A
1	1	2738	A
1	1	2742	C
1	1	2753	G
1	1	2755	C
1	1	2756	C
1	1	2765	C
1	1	2766	U
1	1	2771	U
1	1	2773	C
1	1	2777	G
1	1	2778	G
1	1	2780	A
1	1	2791	G
1	1	2794	G
1	1	2804	A
1	1	2810	C
1	1	2814	G
1	1	2823	G
1	1	2824	G
1	1	2826	U
1	1	2834	G
1	1	2838	A
1	1	2841	G
1	1	2842	U
1	1	2843	U
1	1	2844	C

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Mol	Chain	Res	Type
1	1	2845	A
1	1	2859	U
1	1	2860	U
1	1	2861	U
1	1	2864	A
1	1	2866	U
1	1	2868	U
1	1	2869	U
1	1	2872	A
1	1	2878	G
1	1	2879	C
1	1	2887	A
1	1	2889	C
1	1	2898	G
1	1	2899	C
1	1	2901	G
1	1	2916	U
1	1	2918	G
1	1	2923	U
1	1	2925	C
1	1	2926	A
1	1	2930	A
1	1	2935	U
1	1	2936	A
1	1	2938	G
1	1	2941	A
1	1	2943	G
1	1	2944	U
1	1	2947	G
1	1	2948	C
1	1	2950	G
1	1	2970	C
1	1	2971	A
1	1	2972	G
1	1	2978	U
1	1	2979	U
1	1	2980	U
1	1	2981	U
1	1	2982	A
1	1	2983	C
1	1	2997	G
1	1	3011	A

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Mol	Chain	Res	Type
1	1	3012	A
1	1	3022	G
1	1	3028	G
1	1	3032	A
1	1	3039	C
1	1	3040	A
1	1	3041	U
1	1	3042	U
1	1	3058	U
1	1	3059	G
1	1	3078	U
1	1	3080	G
1	1	3086	A
1	1	3092	C
1	1	3093	C
1	1	3100	U
1	1	3101	G
1	1	3115	C
1	1	3116	G
1	1	3129	A
1	1	3130	A
1	1	3131	U
1	1	3142	A
1	1	3143	C
1	1	3150	A
1	1	3151	U
1	1	3160	U
1	1	3162	C
1	1	3163	A
1	1	3165	A
1	1	3167	A
1	1	3171	U
1	1	3172	A
1	1	3173	G
1	1	3174	A
1	1	3176	G
1	1	3179	U
1	1	3180	A
1	1	3181	C
1	1	3182	G
1	1	3187	A
1	1	3195	U

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Mol	Chain	Res	Type
1	1	3196	U
1	1	3206	C
1	1	3207	U
1	1	3217	C
1	1	3218	A
1	1	3219	G
1	1	3227	A
1	1	3244	A
1	1	3245	A
1	1	3246	G
1	1	3256	G
1	1	3259	U
1	1	3263	G
1	1	3276	G
1	1	3278	C
1	1	3282	U
1	1	3284	G
1	1	3285	C
1	1	3288	G
1	1	3289	G
1	1	3291	G
1	1	3292	A
1	1	3294	A
1	1	3295	A
1	1	3304	U
1	1	3313	U
1	1	3316	A
1	1	3317	U
1	1	3319	U
1	1	3334	U
1	1	3341	U
1	1	3342	A
1	1	3345	G
1	1	3347	A
1	1	3357	U
1	1	3369	G
1	1	3375	A
1	1	3378	C
1	1	3382	U
2	2	25	G
2	2	34	U
2	2	35	C

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Mol	Chain	Res	Type
2	2	49	G
2	2	52	A
2	2	53	A
2	2	59	A
2	2	60	U
2	2	62	C
2	2	63	G
2	2	75	G
2	2	79	A
2	2	81	U
2	2	86	U
2	2	88	A
2	2	90	U
2	2	95	G
2	2	104	A
2	2	106	C
2	2	111	A
2	2	112	U
2	2	113	U
2	2	123	G
2	2	124	G
2	2	126	A
2	2	148	G
2	2	151	C
3	3	7	G
3	3	11	A
3	3	22	A
3	3	35	C
3	3	38	U
3	3	41	G
3	3	49	G
3	3	50	U
3	3	52	G
3	3	53	U
3	3	54	U
3	3	55	A
3	3	64	A
3	3	65	G
3	3	74	C
3	3	99	G
3	3	102	A
3	3	112	G

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Mol	Chain	Res	Type
3	3	121	U

All (28) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	13	A
1	1	40	A
1	1	160	G
1	1	239	G
1	1	784	A
1	1	916	G
1	1	990	U
1	1	1128	U
1	1	1302	A
1	1	1307	G
1	1	1329	U
1	1	1899	G
1	1	2101	C
1	1	2248	C
1	1	2318	U
1	1	2338	C
1	1	2339	C
1	1	2444	C
1	1	2472	U
1	1	2537	U
1	1	2541	U
1	1	2651	G
1	1	2900	A
1	1	3041	U
1	1	3042	U
1	1	3166	C
2	2	123	G
3	3	52	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 6 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
57	GTP	m	501	58	33,34,34	0.87	0	50,54,54	1.55	9 (18%)
57	GTP	b	701	58	33,34,34	0.94	1 (3%)	50,54,54	1.65	8 (16%)

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
57	GTP	m	501	58	-	6/22/38/38	0/3/3/3
57	GTP	b	701	58	-	1/22/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	b	701	GTP	C2-N3	2.27	1.38	1.33

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	b	701	GTP	C5-C4-N3	-5.20	120.12	128.39
57	m	501	GTP	C5-C4-N3	-4.85	120.67	128.39
57	b	701	GTP	C2-N3-C4	4.61	120.24	112.30
57	m	501	GTP	C2-N3-C4	4.50	120.05	112.30
57	b	701	GTP	N9-C4-N3	3.47	132.89	125.95
57	b	701	GTP	C2-N1-C6	-3.16	119.38	125.11
57	m	501	GTP	C2-N1-C6	-3.02	119.63	125.11
57	m	501	GTP	N9-C4-N3	2.88	131.72	125.95
57	m	501	GTP	N9-C8-N7	-2.78	108.24	113.40
57	b	701	GTP	N9-C8-N7	-2.78	108.24	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	b	701	GTP	O6-C6-C5	-2.70	119.40	126.53
57	b	701	GTP	C5-C6-N1	2.62	119.91	113.25
57	m	501	GTP	C8-N7-C5	2.60	108.89	104.26
57	b	701	GTP	C8-N7-C5	2.58	108.86	104.26
57	m	501	GTP	C5-C6-N1	2.48	119.57	113.25
57	m	501	GTP	O6-C6-C5	-2.35	120.34	126.53
57	m	501	GTP	O2B-PB-O3A	2.06	112.84	107.27

There are no chirality outliers.

All (7) torsion outliers are listed below:

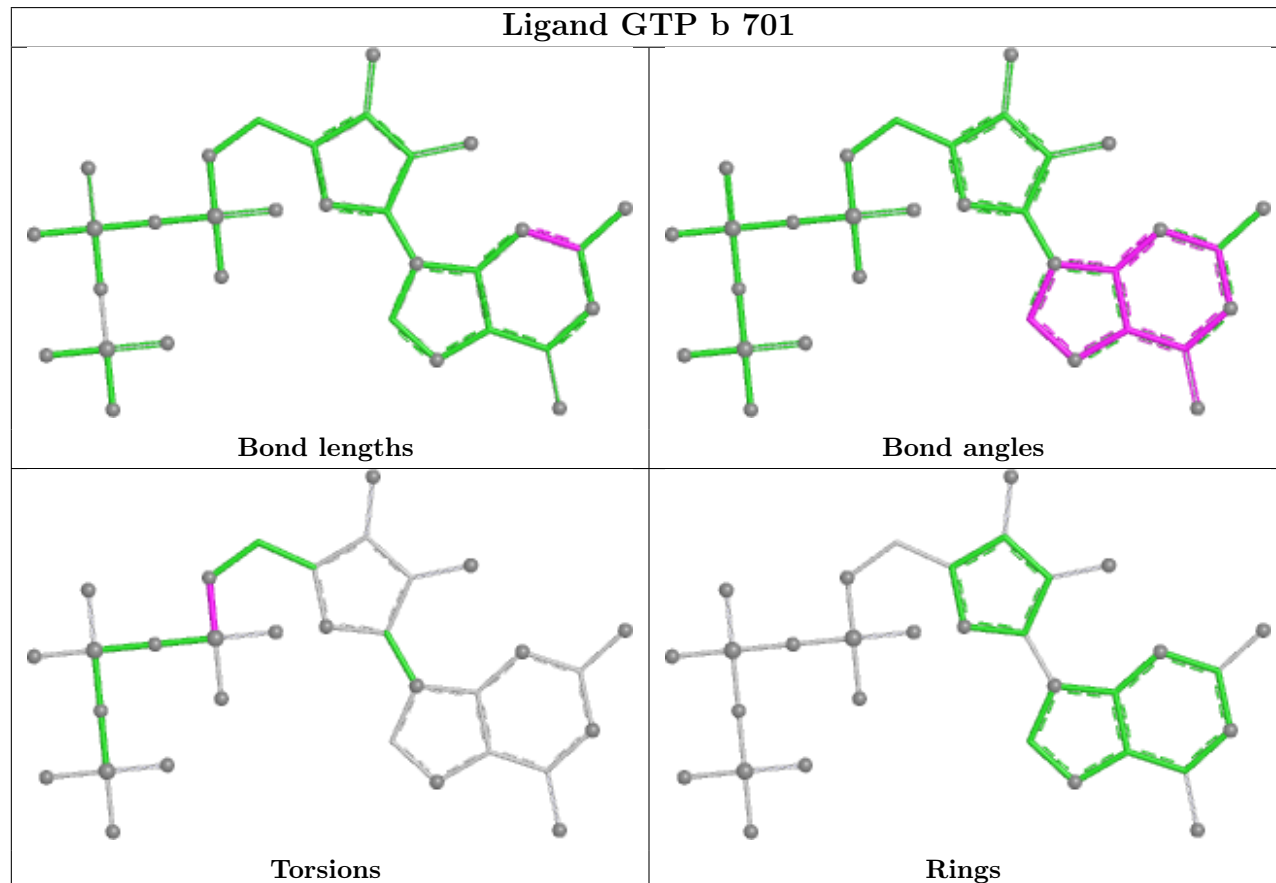
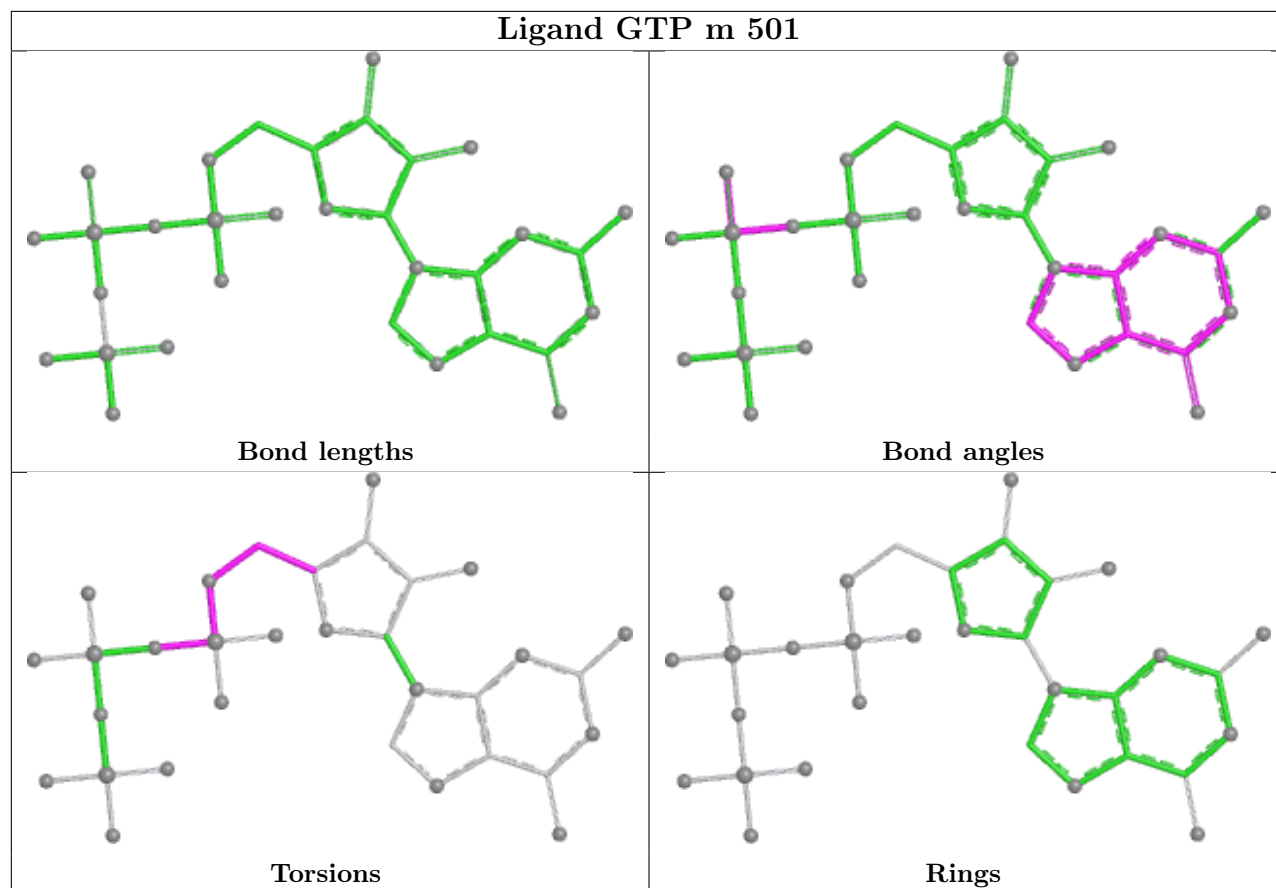
Mol	Chain	Res	Type	Atoms
57	b	701	GTP	C5'-O5'-PA-O1A
57	m	501	GTP	C5'-O5'-PA-O3A
57	m	501	GTP	C5'-O5'-PA-O2A
57	m	501	GTP	O4'-C4'-C5'-O5'
57	m	501	GTP	C3'-C4'-C5'-O5'
57	m	501	GTP	PB-O3A-PA-O1A
57	m	501	GTP	C4'-C5'-O5'-PA

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	m	501	GTP	3	0
57	b	701	GTP	2	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	3167:A	O3'	3168:A	P	4.92
1	1	1012:G	O3'	1013:G	P	3.13
1	1	1039:U	O3'	1040:A	P	3.07

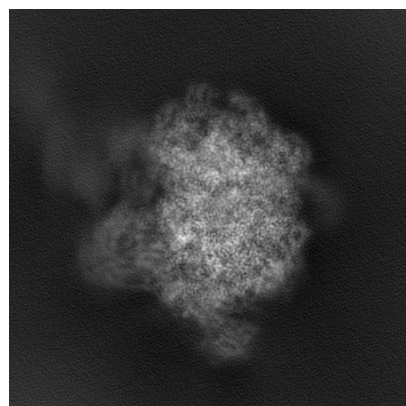
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10838. These allow visual inspection of the internal detail of the map and identification of artifacts.

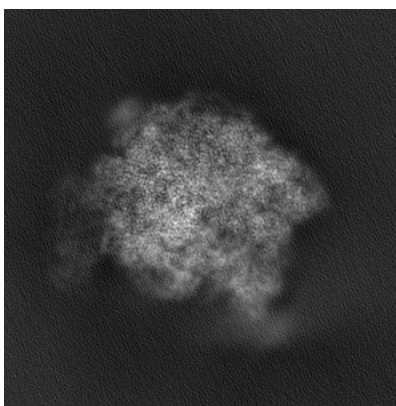
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

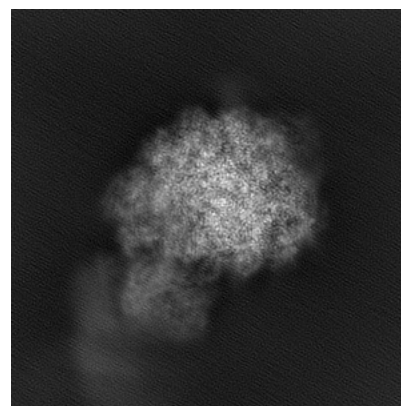
6.1.1 Primary map



X

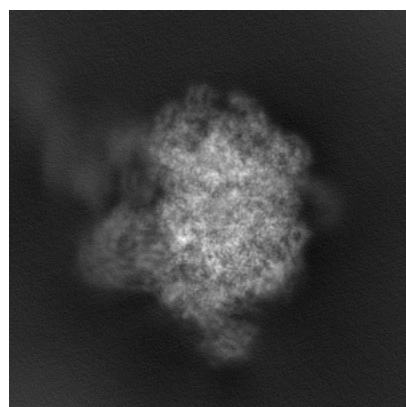


Y

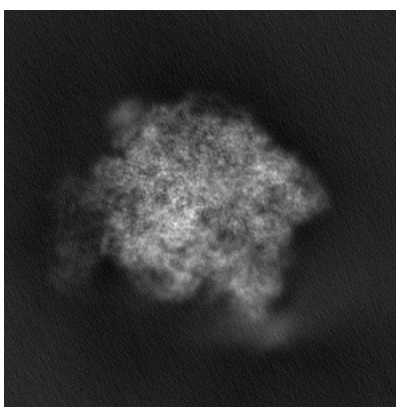


Z

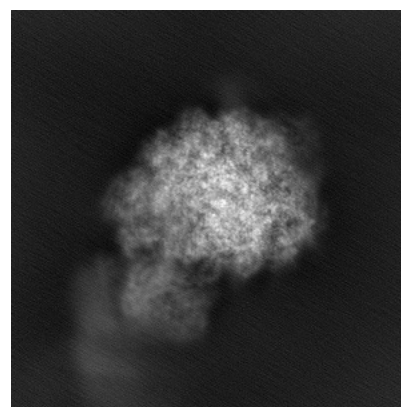
6.1.2 Raw map



X



Y

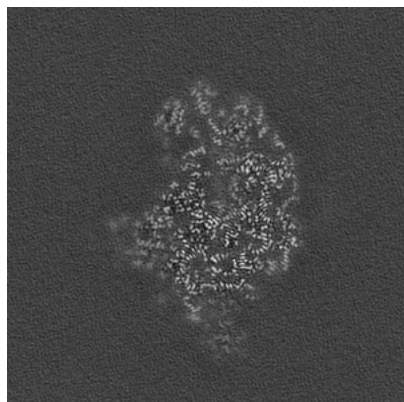


Z

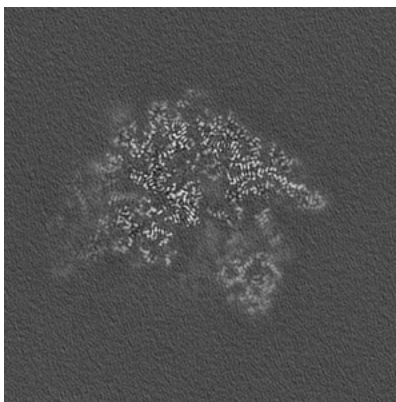
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

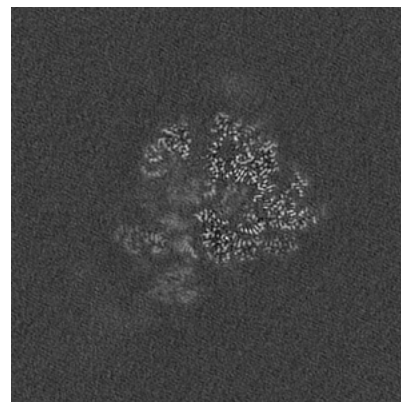
6.2.1 Primary map



X Index: 200

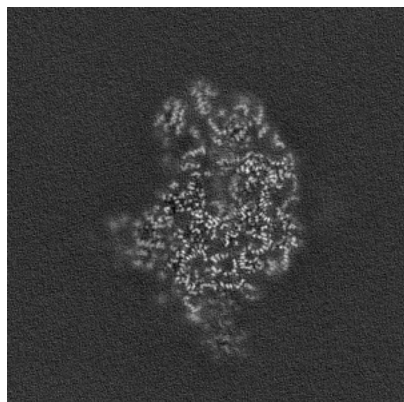


Y Index: 200

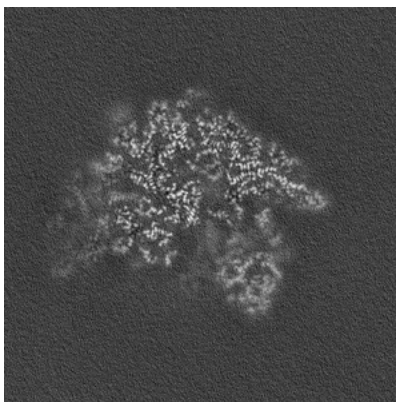


Z Index: 200

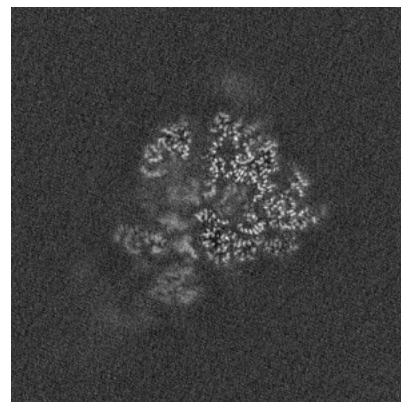
6.2.2 Raw map



X Index: 200



Y Index: 200

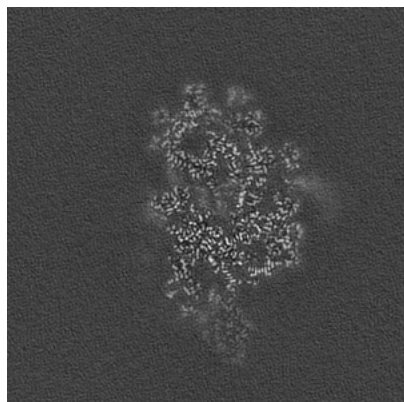


Z Index: 200

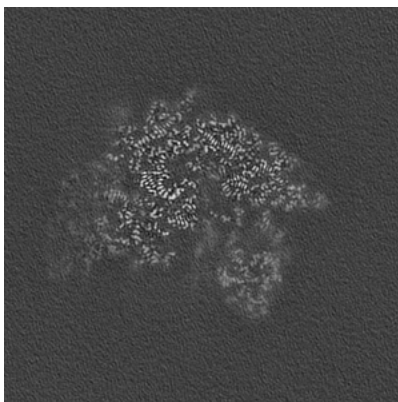
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

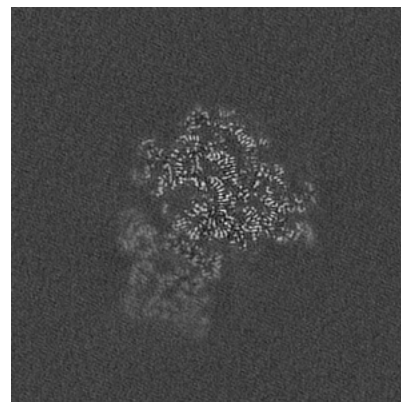
6.3.1 Primary map



X Index: 216

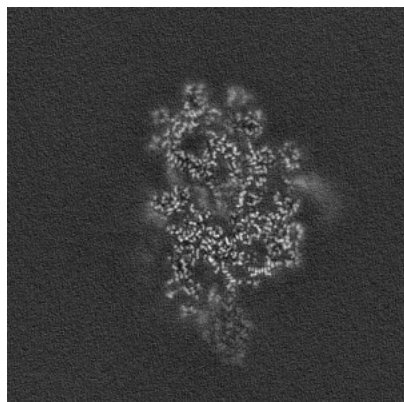


Y Index: 203

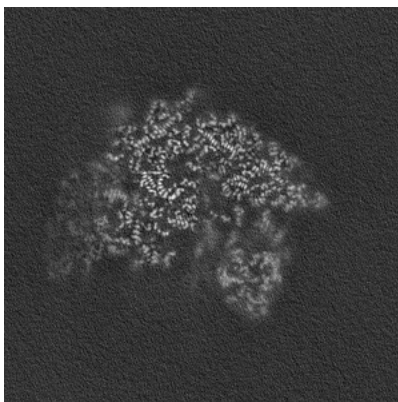


Z Index: 171

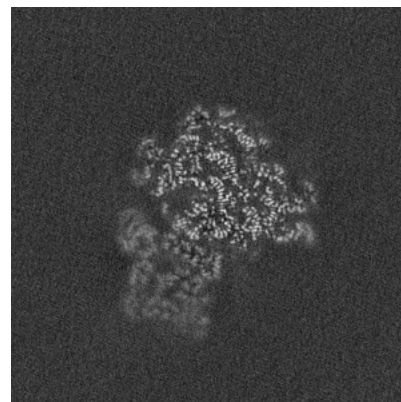
6.3.2 Raw map



X Index: 216



Y Index: 203

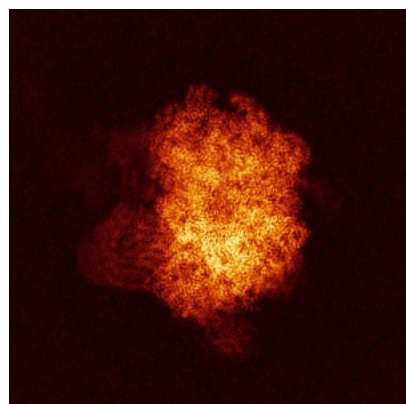


Z Index: 171

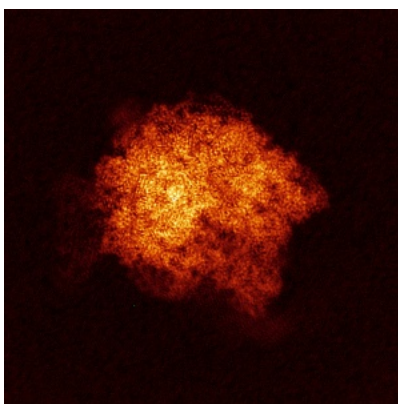
The images above show the largest variance slices of the map in three orthogonal directions.

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

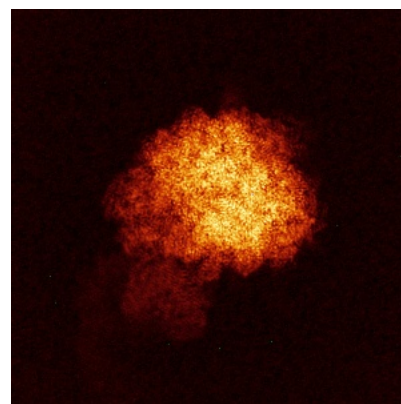
6.4.1 Primary map



X

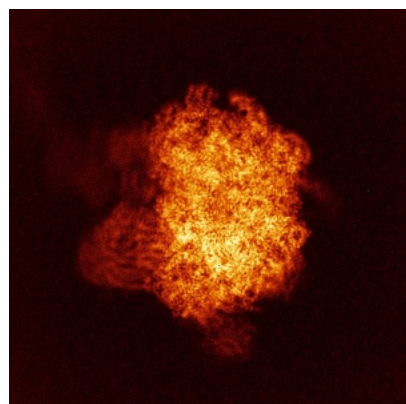


Y

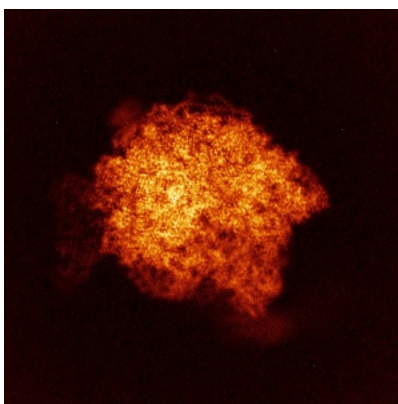


Z

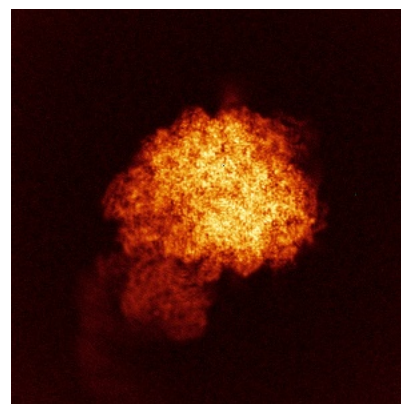
6.4.2 Raw map



X



Y

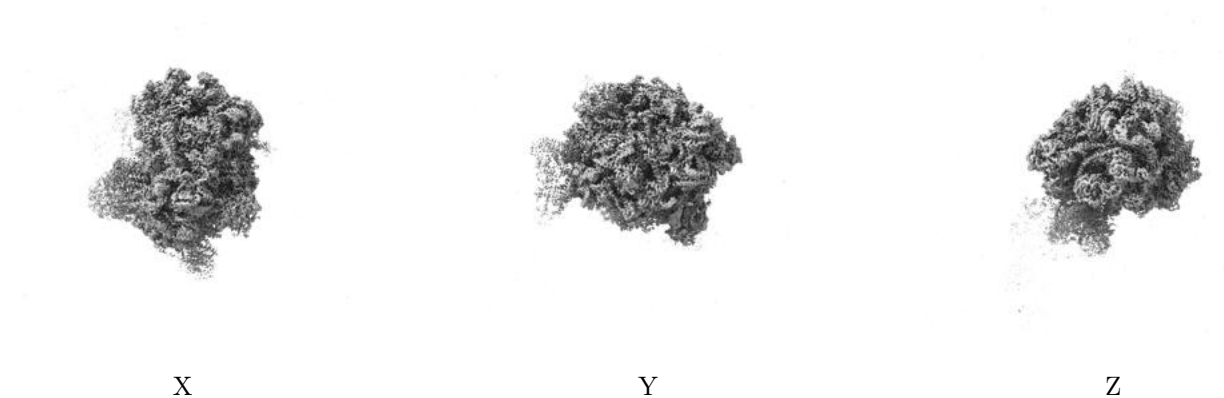


Z

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.

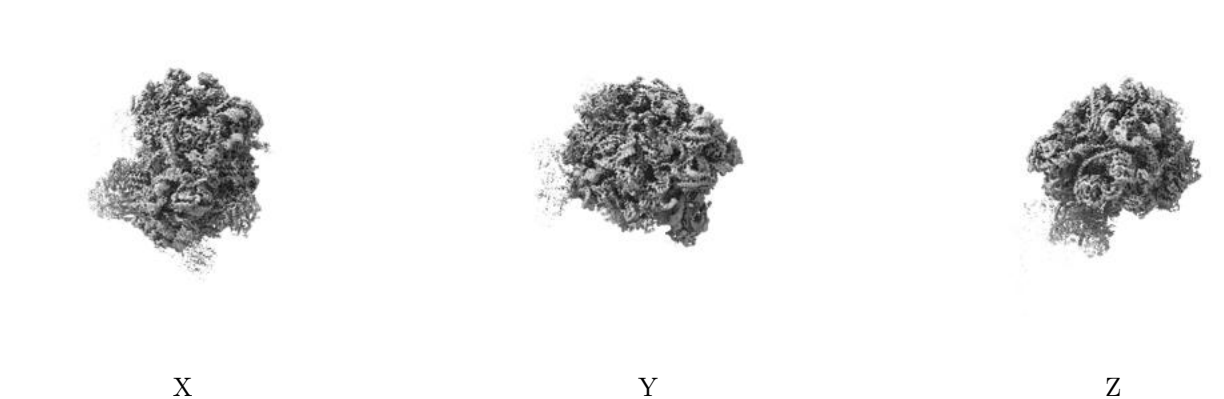
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

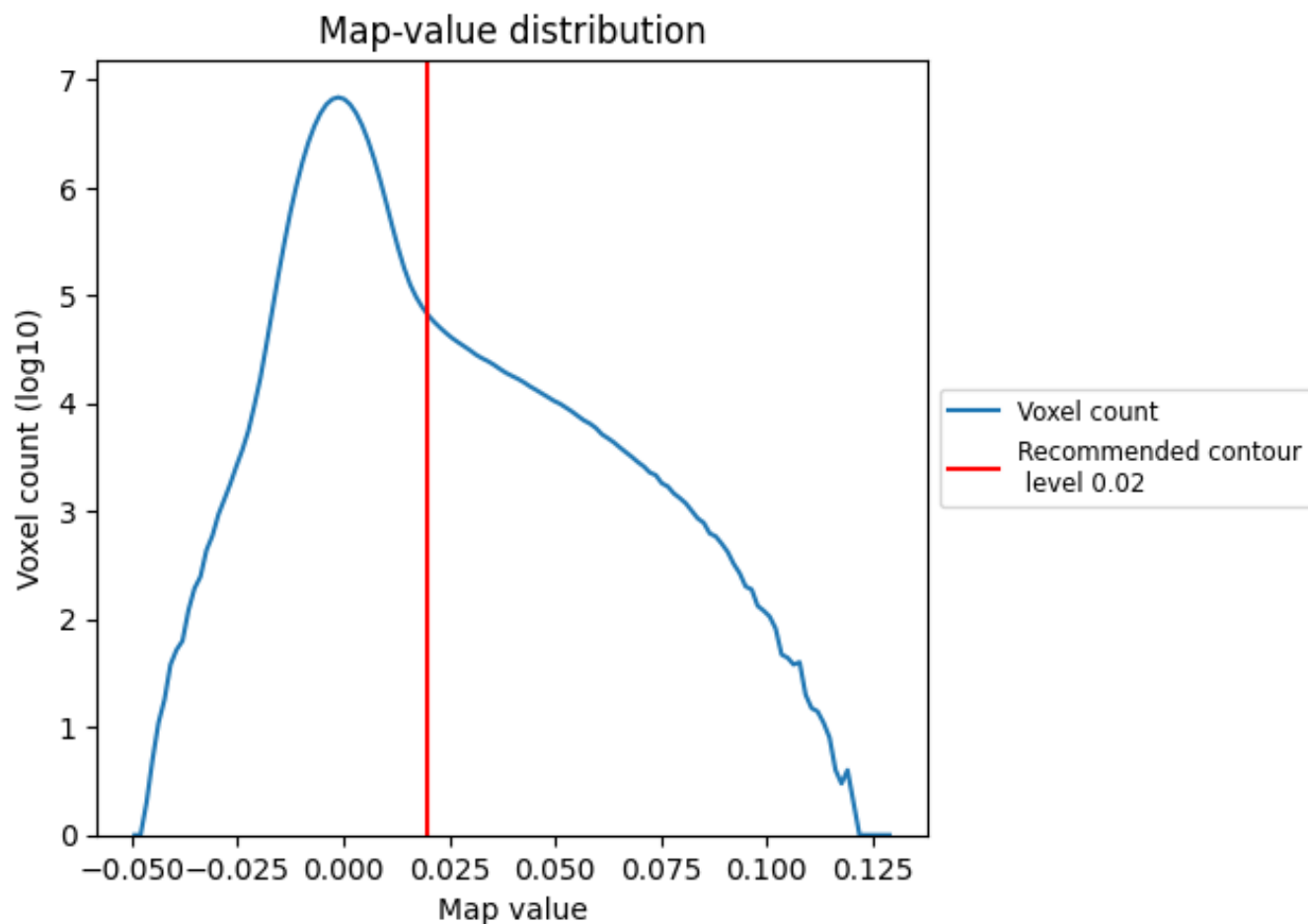
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

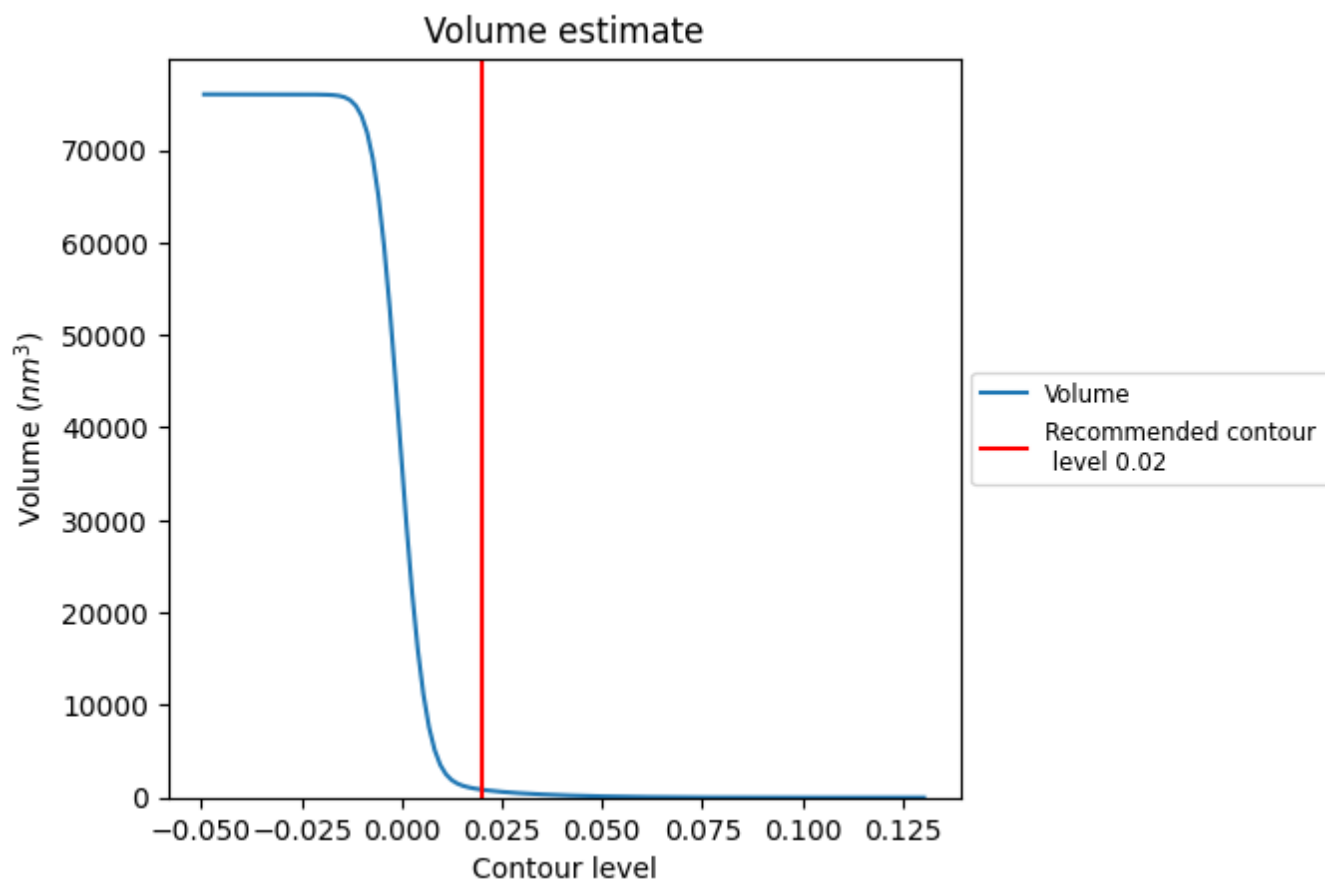
This section contains the results of statistical analysis of the map.

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.

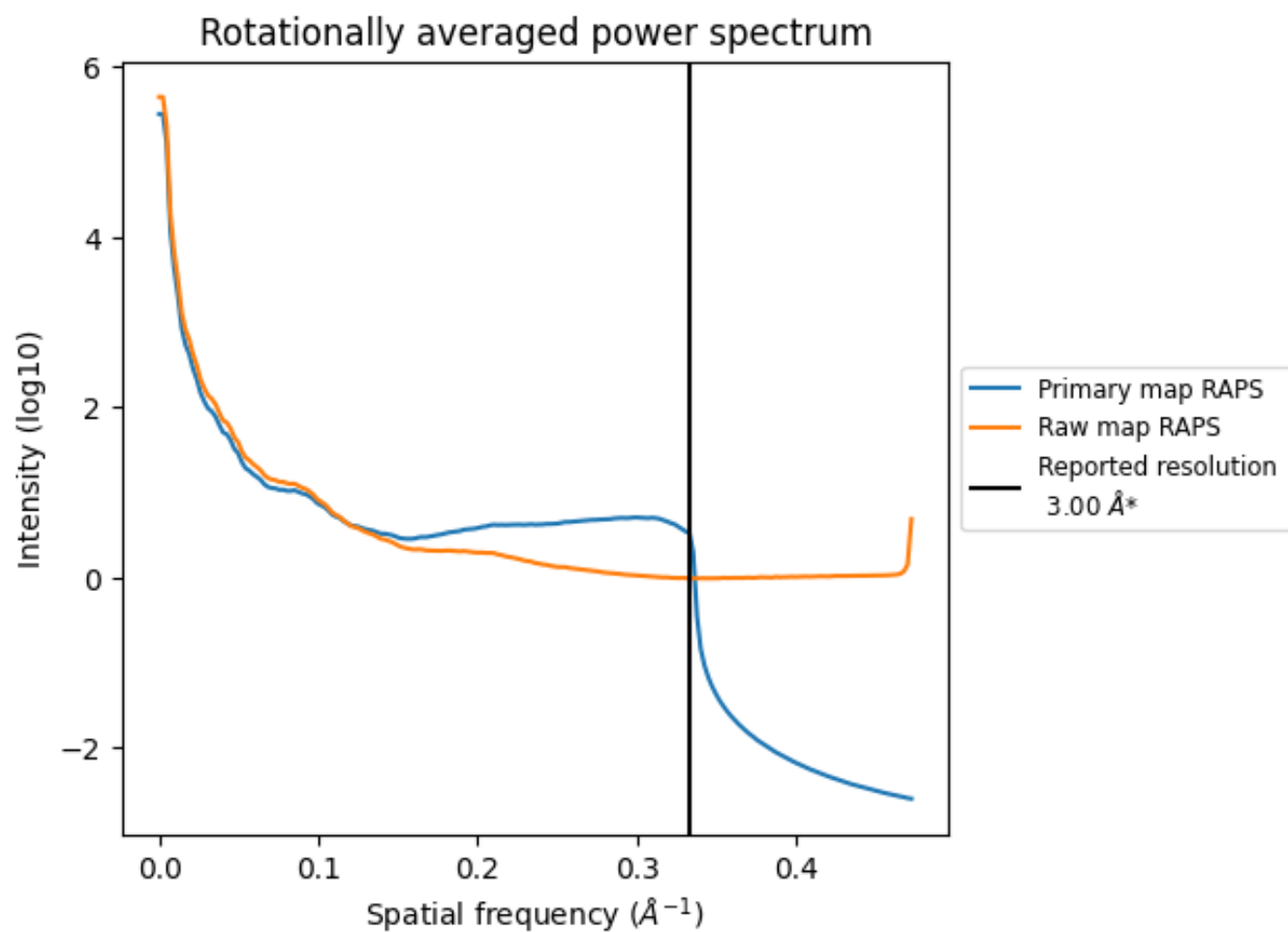
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 856 nm³; this corresponds to an approximate mass of 773 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 ⓘ

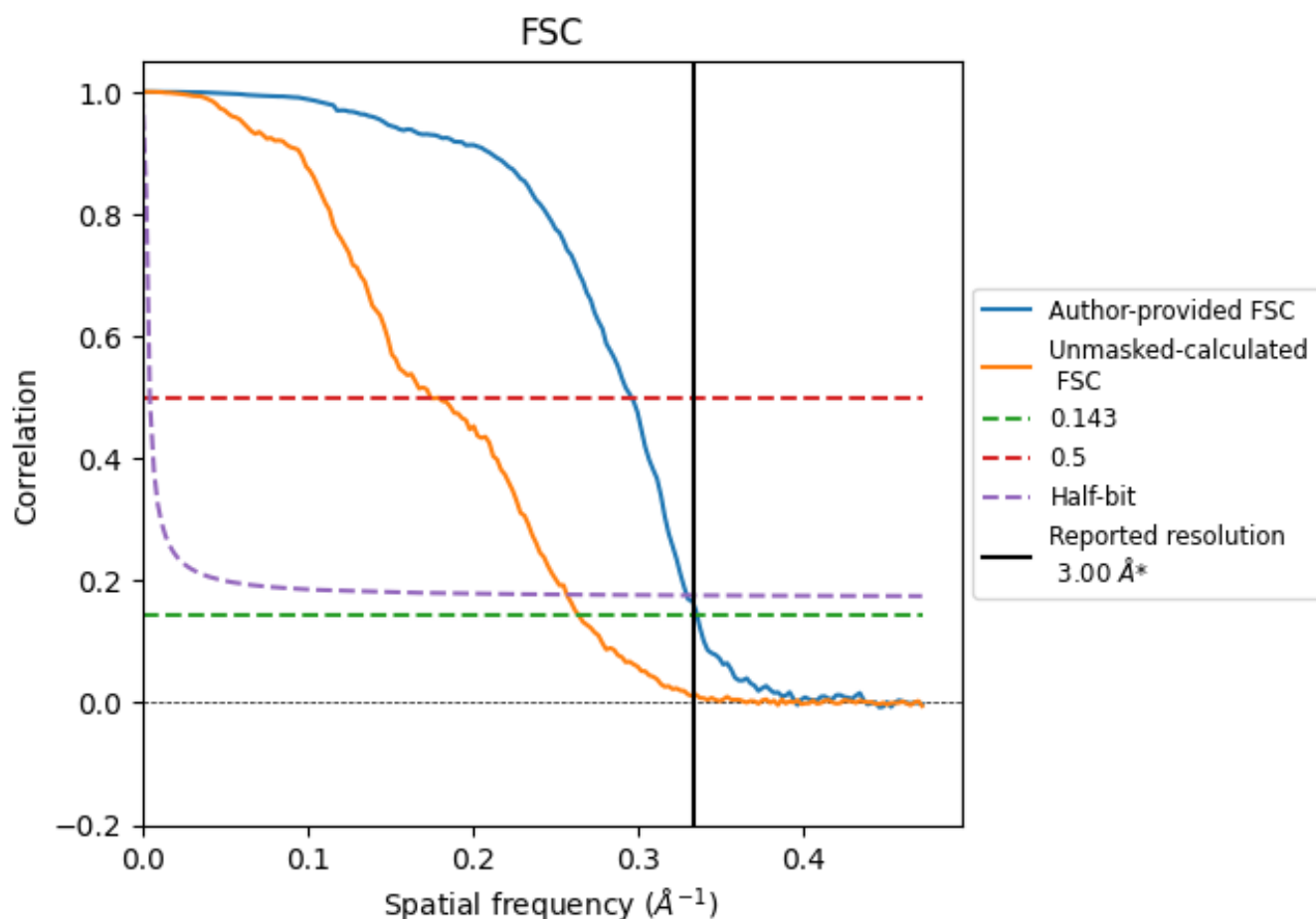


*Reported resolution corresponds to spatial frequency of 0.333 $\text{\AA}^{-1}$

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 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

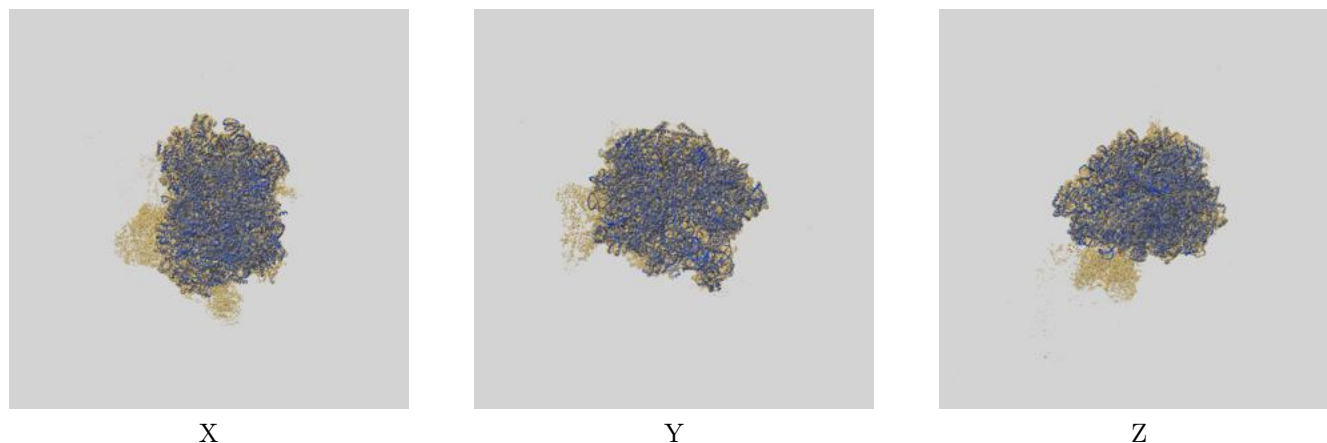
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.98	3.38	3.03
Unmasked-calculated*	3.79	5.73	3.89

*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 3.79 differs from the reported value 3.0 by more than 10 %

9 Map-model fit [i](#)

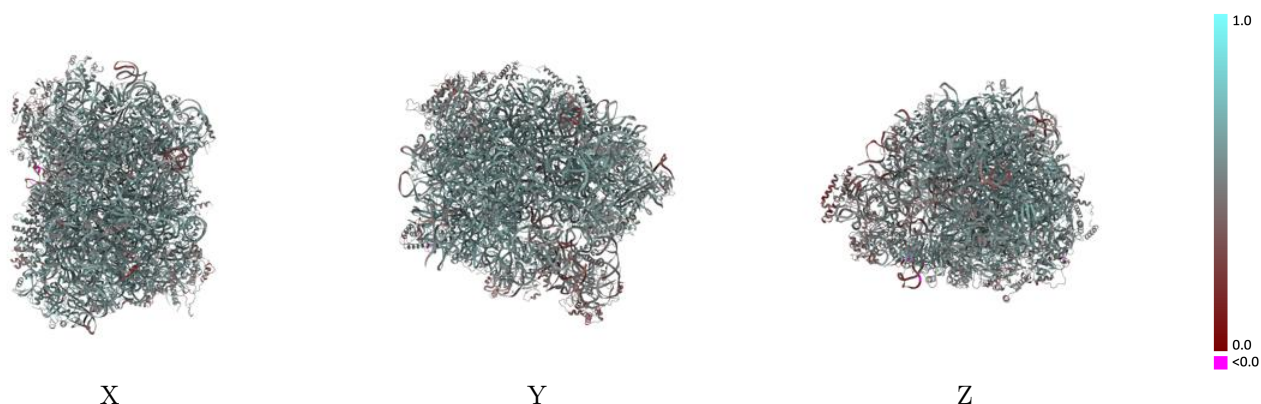
This section contains information regarding the fit between EMDB map EMD-10838 and PDB model 6YLG. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



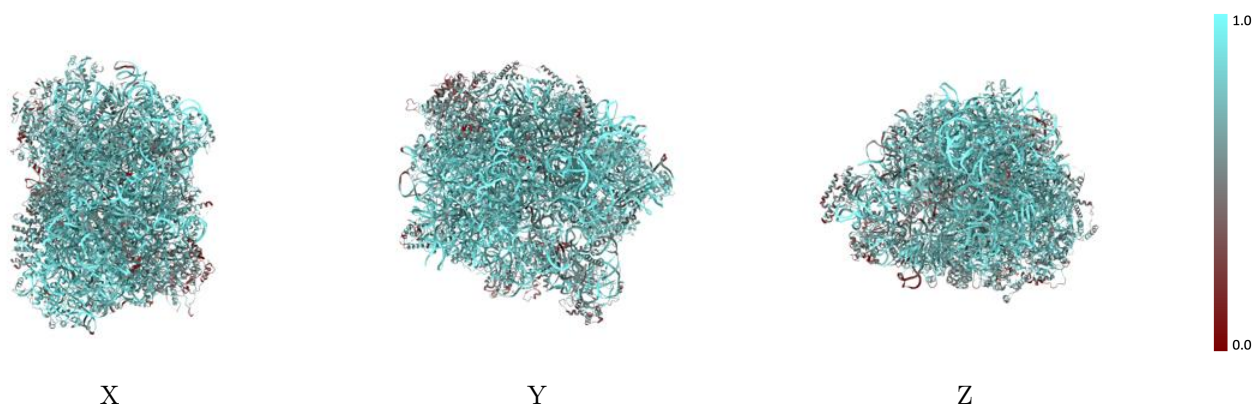
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



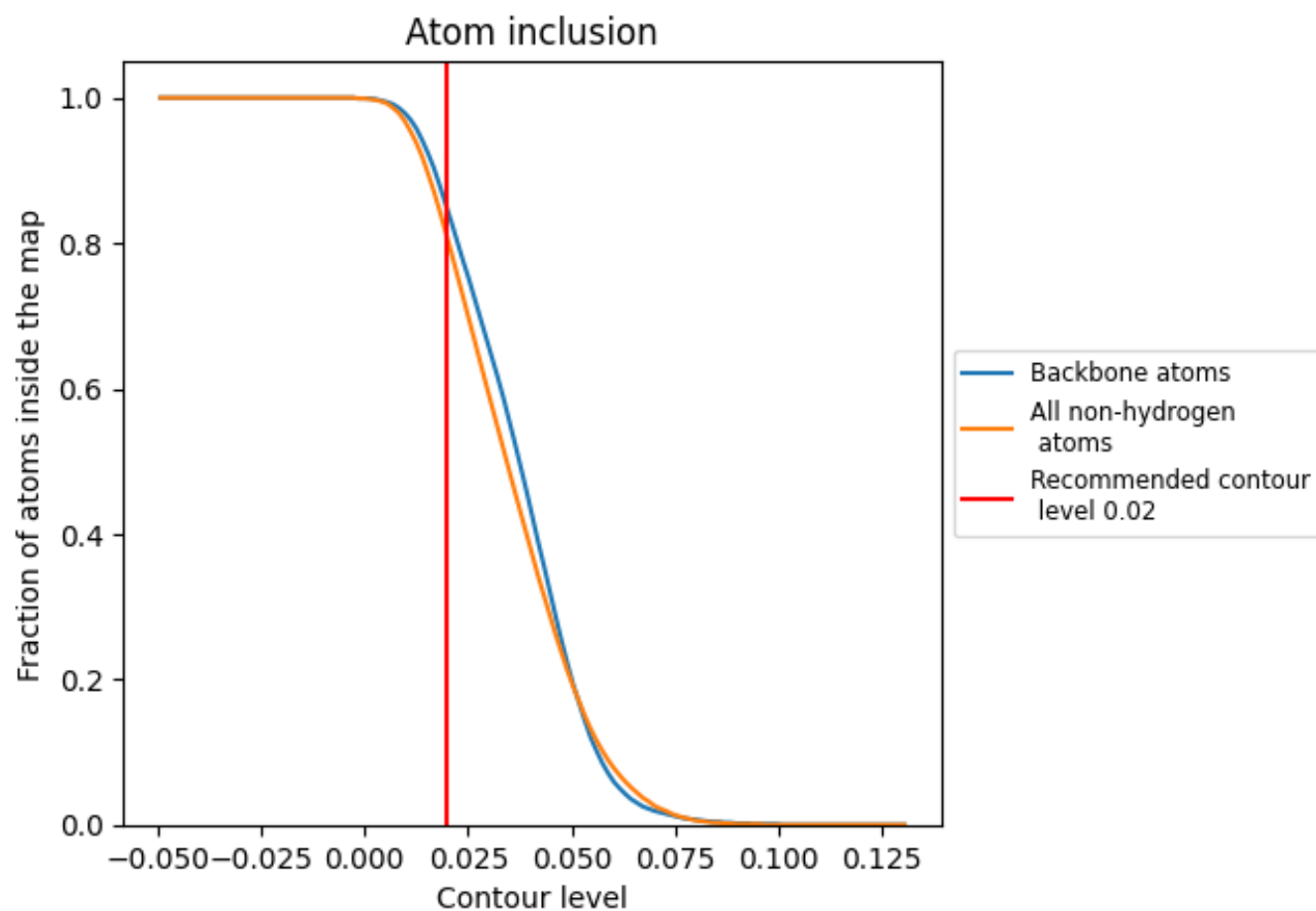
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 81% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8060	 0.5450
1	 0.8930	 0.5550
2	 0.9410	 0.5890
3	 0.8600	 0.4940
4	 0.5350	 0.4960
5	 0.5110	 0.4530
A	 0.8680	 0.6000
B	 0.8140	 0.5750
C	 0.8000	 0.5680
D	 0.5290	 0.4160
E	 0.7600	 0.5430
F	 0.7970	 0.5550
G	 0.7490	 0.5330
H	 0.7890	 0.5620
I	 0.6210	 0.5320
J	 0.6060	 0.4570
K	 0.6130	 0.4870
L	 0.7890	 0.5520
M	 0.8070	 0.5580
N	 0.8530	 0.5920
O	 0.8290	 0.5790
P	 0.8210	 0.5800
Q	 0.7790	 0.5570
R	 0.8060	 0.5610
S	 0.7420	 0.5420
T	 0.5150	 0.4710
U	 0.7730	 0.5390
V	 0.7460	 0.5110
W	 0.7110	 0.5050
X	 0.7670	 0.5720
Y	 0.7970	 0.5690
Z	 0.7860	 0.5410
a	 0.8120	 0.5640
b	 0.6590	 0.5160
c	 0.5520	 0.5410



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Chain	Atom inclusion	Q-score
d	 0.7870	 0.5720
e	 0.8070	 0.5820
f	 0.8540	 0.6020
g	 0.8070	 0.5760
h	 0.8040	 0.5690
i	 0.7500	 0.5420
j	 0.8830	 0.6000
k	 0.6910	 0.5320
l	 0.8530	 0.6010
m	 0.7500	 0.5510
n	 0.7850	 0.5390
o	 0.3630	 0.3880
p	 0.8140	 0.5820
q	 0.6040	 0.4710
r	 0.7920	 0.5720
s	 0.4980	 0.5050
t	 0.6360	 0.5100
u	 0.7590	 0.5460
x	 0.7530	 0.5360
y	 0.6930	 0.5060
z	 0.6190	 0.5340