Full wwPDB EM Validation Report ⓘ

Jan 7, 2025 – 07:30 pm GMT

PDB ID	:	9FNZ
EMDB ID	:	EMD-50612
Title	:	PF30S-PF30S dimer mediated by aRDF from P. furiosus (Structure II)
Authors	:	Hassan, A.H.; Demo, G.
Deposited on	:	2024-06-11
Resolution	:	3.20 Å(reported)
Based on initial models	:	4V6U, 7ZHG, .

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:

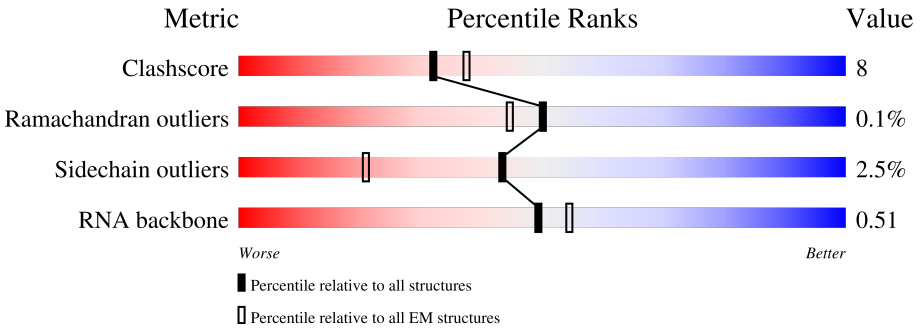
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 Å.

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



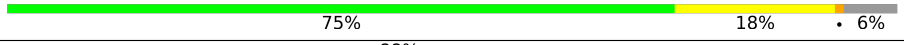
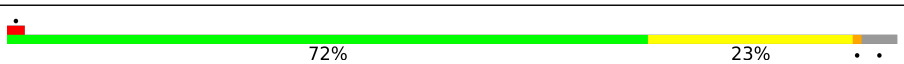
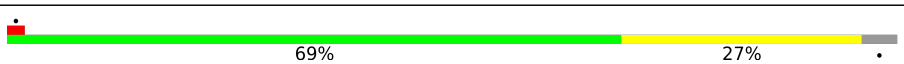
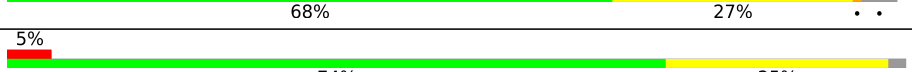
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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 <=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	A1	60	10% 78% 20%
1	B1	60	7% 77% 22%
2	A2	37	51% 43% 5%
2	B2	37	68% 27% 5%
3	A3	306	70% 27%
3	A4	306	72% 22% 5%
3	B3	306	73% 24%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	B4	306	
4	A5	123	
4	B5	123	
5	AA	1495	
5	BA	1495	
6	AB	202	
6	BB	202	
7	AC	210	
7	BC	210	
8	AD	198	
8	BD	198	
9	AE	180	
9	BE	180	
10	AF	243	
10	BF	243	
11	AG	236	
11	BG	236	
12	AH	125	
12	BH	125	
13	AI	215	
13	BI	215	
14	AJ	130	
14	BJ	130	
15	AK	127	
15	BK	127	

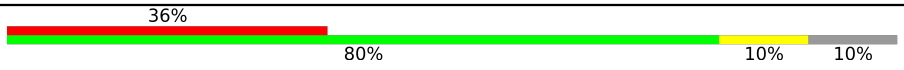
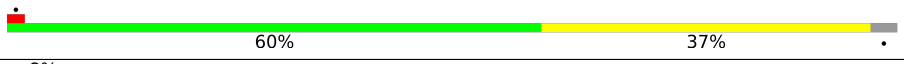
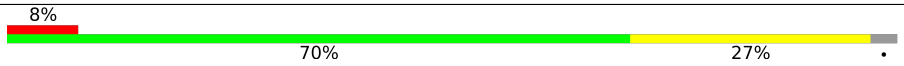
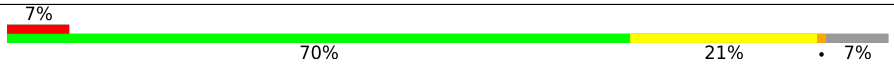
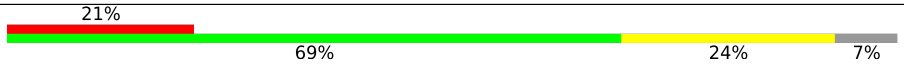
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
16	AL	135	24% 81% 13% 5%
16	BL	135	17% 79% 16% 5%
17	AM	102	28% 82% 18%
17	BM	102	23% 75% 23%
18	AN	137	79% 13% 7%
18	BN	137	75% 18% 7%
19	AO	147	77% 20%
19	BO	147	82% 14%
20	AP	148	46% 64% 25% 11%
20	BP	148	57% 62% 25% 11%
21	AQ	56	9% 77% 12% 11%
21	BQ	56	23% 66% 23% 11%
22	AR	158	68% 29%
22	BR	158	77% 21%
23	AS	113	58% 38%
23	BS	113	74% 23%
24	AT	67	7% 69% 22% 6%
24	BT	67	66% 27% 6%
25	AU	132	64% 66% 21% 13%
25	BU	132	64% 70% 17% 13%
26	AV	150	26% 84% 15%
26	BV	150	14% 75% 23%
27	AW	99	7% 64% 28% 6%
27	BW	99	64% 30% 6%
28	AX	50	32% 76% 12% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	BX	50	
29	AY	63	
29	BY	63	
30	AZ	71	
30	BZ	71	

2 Entry composition (i)

There are 30 unique types of molecules in this entry. The entry contains 130980 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called RNA-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A1	60	Total	C	N	O	S	0	0
			471	295	83	83	10		
1	B1	60	Total	C	N	O	S	0	0
			471	295	83	83	10		

- Molecule 2 is a protein called Small ribosomal subunit protein eS32.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A2	35	Total	C	N	O	S	0	0
			335	212	83	38	2		
2	B2	35	Total	C	N	O	S	0	0
			335	212	83	38	2		

- Molecule 3 is a protein called Archaeal Ribosome Dimerizing Factor (aRDF).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A3	298	Total	C	N	O	S	0	0
			2375	1537	395	439	4		
3	A4	291	Total	C	N	O	S	0	0
			2321	1503	387	427	4		
3	B3	299	Total	C	N	O	S	0	0
			2381	1540	396	441	4		
3	B4	289	Total	C	N	O	S	0	0
			2301	1491	381	425	4		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A3	301	HIS	-	expression tag	UNP Q8U3B0
A3	302	HIS	-	expression tag	UNP Q8U3B0
A3	303	HIS	-	expression tag	UNP Q8U3B0
A3	304	HIS	-	expression tag	UNP Q8U3B0
A3	305	HIS	-	expression tag	UNP Q8U3B0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A3	306	HIS	-	expression tag	UNP Q8U3B0
A4	301	HIS	-	expression tag	UNP Q8U3B0
A4	302	HIS	-	expression tag	UNP Q8U3B0
A4	303	HIS	-	expression tag	UNP Q8U3B0
A4	304	HIS	-	expression tag	UNP Q8U3B0
A4	305	HIS	-	expression tag	UNP Q8U3B0
A4	306	HIS	-	expression tag	UNP Q8U3B0
B3	301	HIS	-	expression tag	UNP Q8U3B0
B3	302	HIS	-	expression tag	UNP Q8U3B0
B3	303	HIS	-	expression tag	UNP Q8U3B0
B3	304	HIS	-	expression tag	UNP Q8U3B0
B3	305	HIS	-	expression tag	UNP Q8U3B0
B3	306	HIS	-	expression tag	UNP Q8U3B0
B4	301	HIS	-	expression tag	UNP Q8U3B0
B4	302	HIS	-	expression tag	UNP Q8U3B0
B4	303	HIS	-	expression tag	UNP Q8U3B0
B4	304	HIS	-	expression tag	UNP Q8U3B0
B4	305	HIS	-	expression tag	UNP Q8U3B0
B4	306	HIS	-	expression tag	UNP Q8U3B0

- Molecule 4 is a protein called Large ribosomal subunit protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A5	123	Total	C	N	O	S	0	0
			939	599	155	181	4		
4	B5	123	Total	C	N	O	S	0	0
			939	599	155	181	4		

- Molecule 5 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AA	1495	Total	C	N	O	P	0	0
			32135	14297	5954	10389	1495		
5	BA	1495	Total	C	N	O	P	0	0
			32135	14297	5954	10389	1495		

- Molecule 6 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AB	197	Total	C	N	O	S	0	0
			1579	1022	271	282	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
6	BB	197	Total	C	N	O	S	0	0
			1579	1022	271	282	4		

- Molecule 7 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AC	195	Total	C	N	O	S	0	0
			1532	980	283	266	3		
7	BC	195	Total	C	N	O	S	0	0
			1532	980	283	266	3		

- Molecule 8 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AD	184	Total	C	N	O	S	0	0
			1511	978	263	265	5		
8	BD	184	Total	C	N	O	S	0	0
			1511	978	263	265	5		

- Molecule 9 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AE	173	Total	C	N	O	S	0	0
			1455	915	282	254	4		
9	BE	173	Total	C	N	O	S	0	0
			1455	915	282	254	4		

- Molecule 10 is a protein called Small ribosomal subunit protein eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AF	242	Total	C	N	O	S	0	0
			1981	1280	356	340	5		
10	BF	242	Total	C	N	O	S	0	0
			1981	1280	356	340	5		

- Molecule 11 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AG	227	Total	C	N	O	S	0	0
			1794	1134	335	318	7		
11	BG	227	Total	C	N	O	S	0	0
			1794	1134	335	318	7		

- Molecule 12 is a protein called Small ribosomal subunit protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AH	123	Total	C	N	O	S	0	0
			971	615	178	177	1		
12	BH	123	Total	C	N	O	S	0	0
			971	615	178	177	1		

- Molecule 13 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AI	214	Total	C	N	O	S	0	0
			1728	1095	325	301	7		
13	BI	214	Total	C	N	O	S	0	0
			1728	1095	325	301	7		

- Molecule 14 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AJ	129	Total	C	N	O	S	0	0
			1028	668	178	180	2		
14	BJ	129	Total	C	N	O	S	0	0
			1028	668	178	180	2		

- Molecule 15 is a protein called Small ribosomal subunit protein eS8.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	AK	124	Total	C	N	O	0	0
			977	607	204	166		
15	BK	124	Total	C	N	O	0	0
			977	607	204	166		

- Molecule 16 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AL	128	Total	C	N	O	S	0	0
			1006	630	191	180	5		
16	BL	128	Total	C	N	O	S	0	0
			1006	630	191	180	5		

- Molecule 17 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AM	102	Total	C	N	O	S	0	0
			822	507	159	152	4		
17	BM	102	Total	C	N	O	S	0	0
			822	507	159	152	4		

- Molecule 18 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AN	127	Total	C	N	O	S	0	0
			954	591	190	171	2		
18	BN	127	Total	C	N	O	S	0	0
			954	591	190	171	2		

- Molecule 19 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AO	143	Total	C	N	O	S	0	0
			1118	710	215	190	3		
19	BO	143	Total	C	N	O	S	0	0
			1118	710	215	190	3		

- Molecule 20 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AP	131	Total	C	N	O	S	0	0
			1052	663	206	178	5		
20	BP	131	Total	C	N	O	S	0	0
			1052	663	206	178	5		

- Molecule 21 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AQ	50	Total	C	N	O	S	0	0
			417	266	88	58	5		
21	BQ	50	Total	C	N	O	S	0	0
			417	266	88	58	5		

- Molecule 22 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AR	155	Total	C	N	O	S	0	0
			1283	818	244	217	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BR	155	Total	C	N	O	S	0	0
			1283	818	244	217	4		

- Molecule 23 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AS	110	Total	C	N	O	S	0	0
			903	575	168	156	4		
23	BS	110	Total	C	N	O	S	0	0
			903	575	168	156	4		

- Molecule 24 is a protein called Small ribosomal subunit protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AT	63	Total	C	N	O	S	0	0
			522	330	100	90	2		
24	BT	63	Total	C	N	O	S	0	0
			522	330	100	90	2		

- Molecule 25 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AU	115	Total	C	N	O	S	0	0
			948	609	177	156	6		
25	BU	115	Total	C	N	O	S	0	0
			948	609	177	156	6		

- Molecule 26 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	AV	148	Total	C	N	O	0	0
			1209	781	218	210		
26	BV	148	Total	C	N	O	0	0
			1209	781	218	210		

- Molecule 27 is a protein called Small ribosomal subunit protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	AW	93	Total	C	N	O	S	0	0
			774	503	126	143	2		
27	BW	93	Total	C	N	O	S	0	0
			774	503	126	143	2		

- Molecule 28 is a protein called Small ribosomal subunit protein eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	AX	45	Total	C	N	O	S	0	0
			369	238	67	59	5		
28	BX	45	Total	C	N	O	S	0	0
			369	238	67	59	5		

- Molecule 29 is a protein called Small ribosomal subunit protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	AY	61	Total	C	N	O	S	0	0
			465	298	83	79	5		
29	BY	61	Total	C	N	O	S	0	0
			465	298	83	79	5		

- Molecule 30 is a protein called Small ribosomal subunit protein eS28.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	AZ	66	Total	C	N	O	0	0
			523	320	104	99		
30	BZ	66	Total	C	N	O	0	0
			523	320	104	99		

3 Residue-property plots (i)

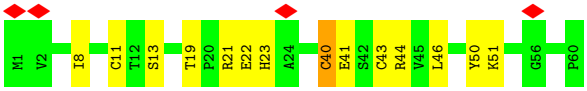
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: RNA-binding protein

Chain A1:

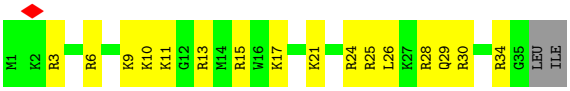
• Molecule 1: RNA-binding protein

Chain B1:



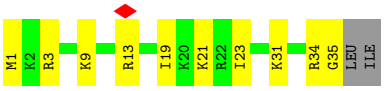
• Molecule 2: Small ribosomal subunit protein eS32

Chain A2:



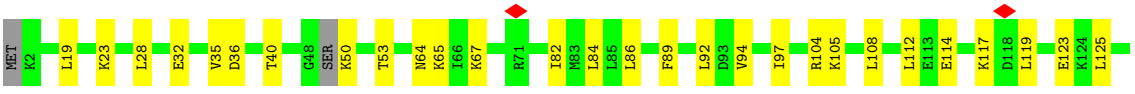
• Molecule 2: Small ribosomal subunit protein eS32

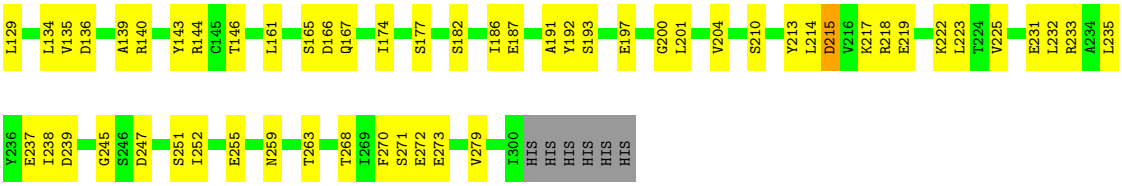
Chain B2:



• Molecule 3: Archaeal Ribosome Dimerizing Factor (aRDF)

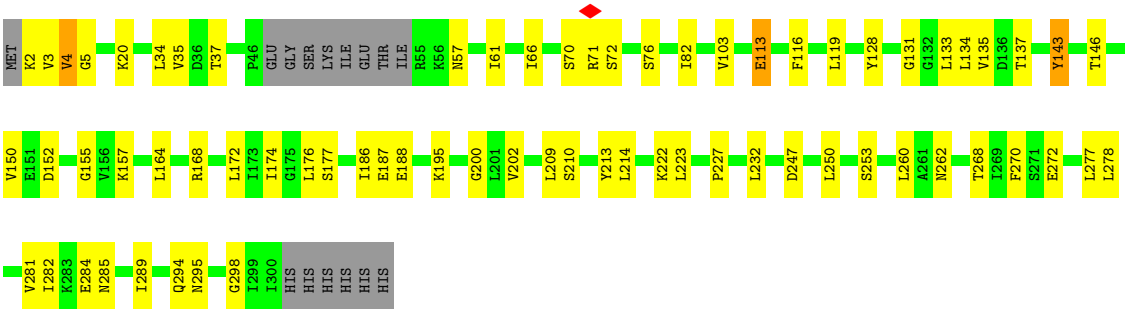
Chain A3:





• Molecule 3: Archaeal Ribosome Dimerizing Factor (aRDF)

Chain A4:

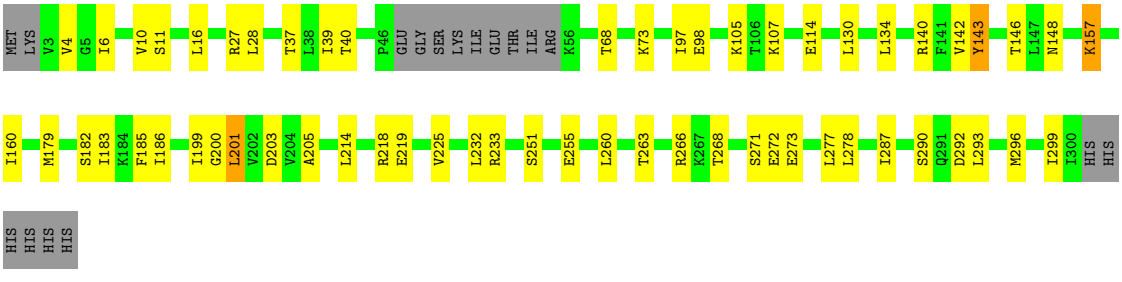


• Molecule 3: Archaeal Ribosome Dimerizing Factor (aRDF)

Chain B3:

• Molecule 3: Archaeal Ribosome Dimerizing Factor (aRDF)

Chain B4:

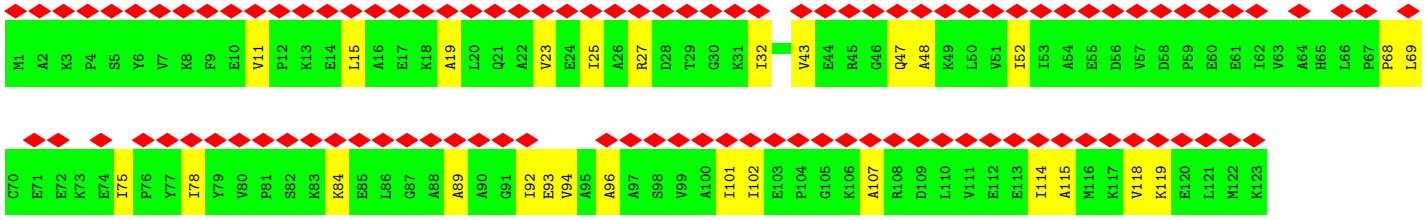


• Molecule 4: Large ribosomal subunit protein eL8

Chain A5:

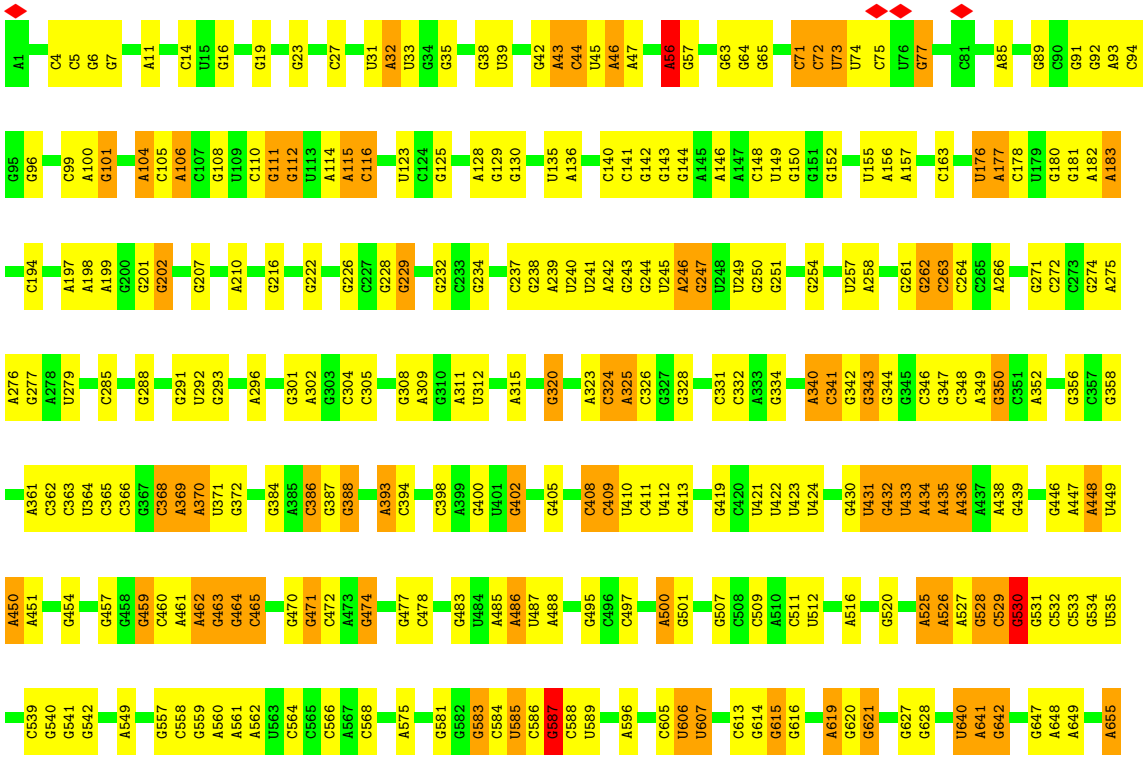
• Molecule 4: Large ribosomal subunit protein eL8

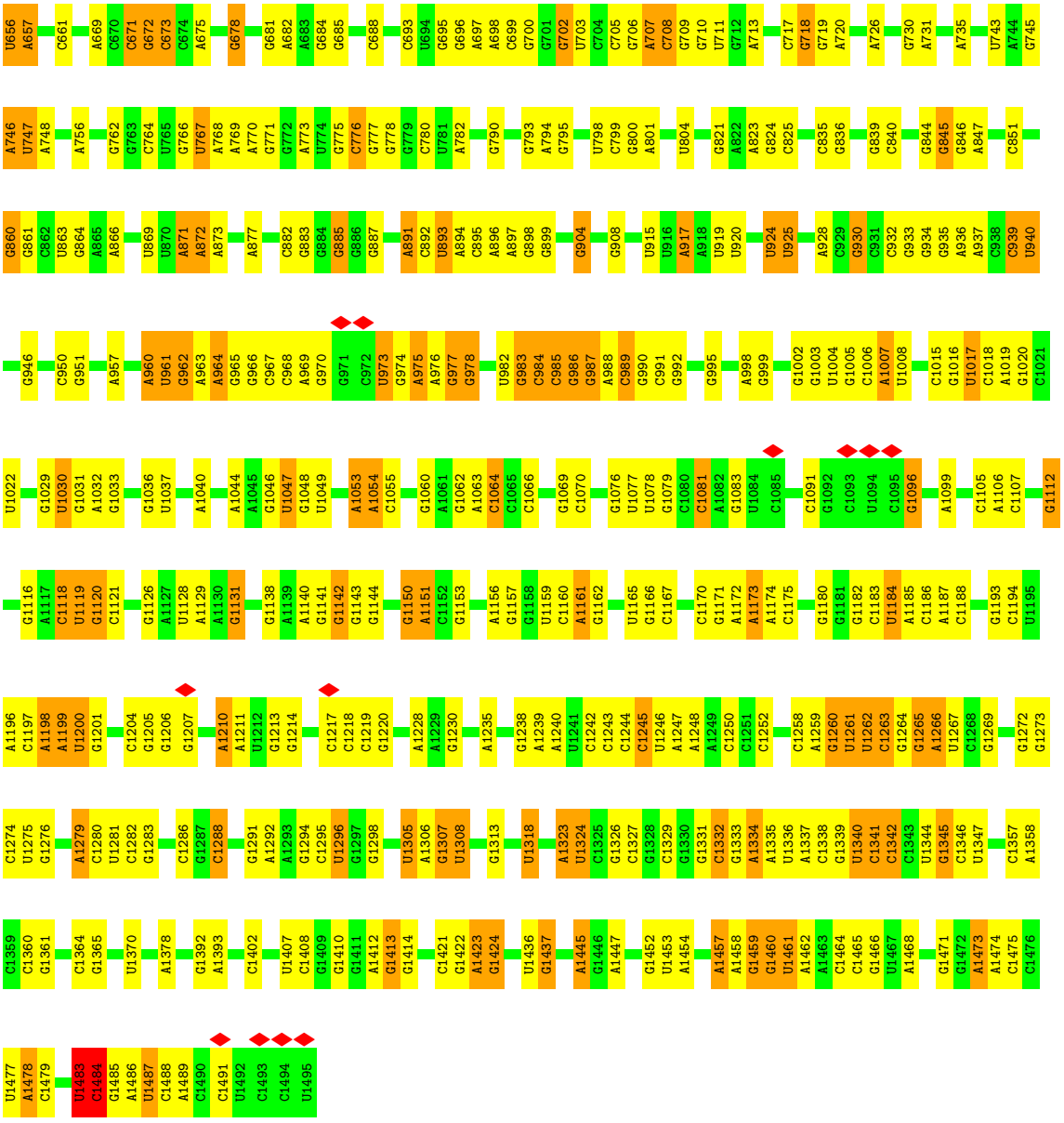
Chain B5:



• Molecule 5: 16S rRNA

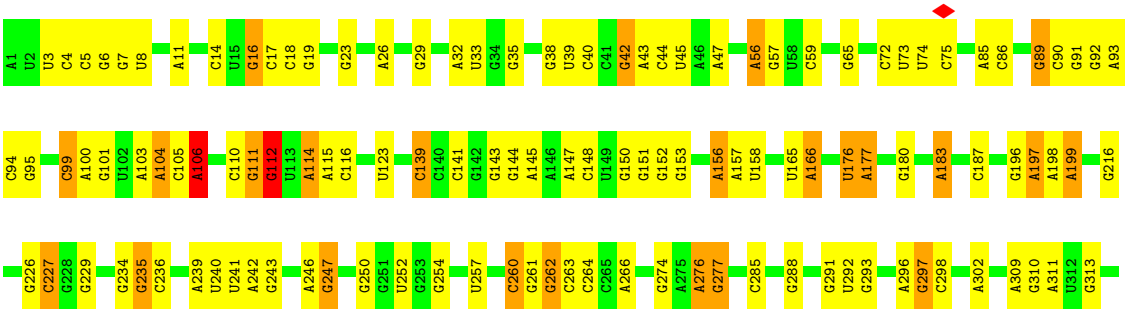
Chain AA:

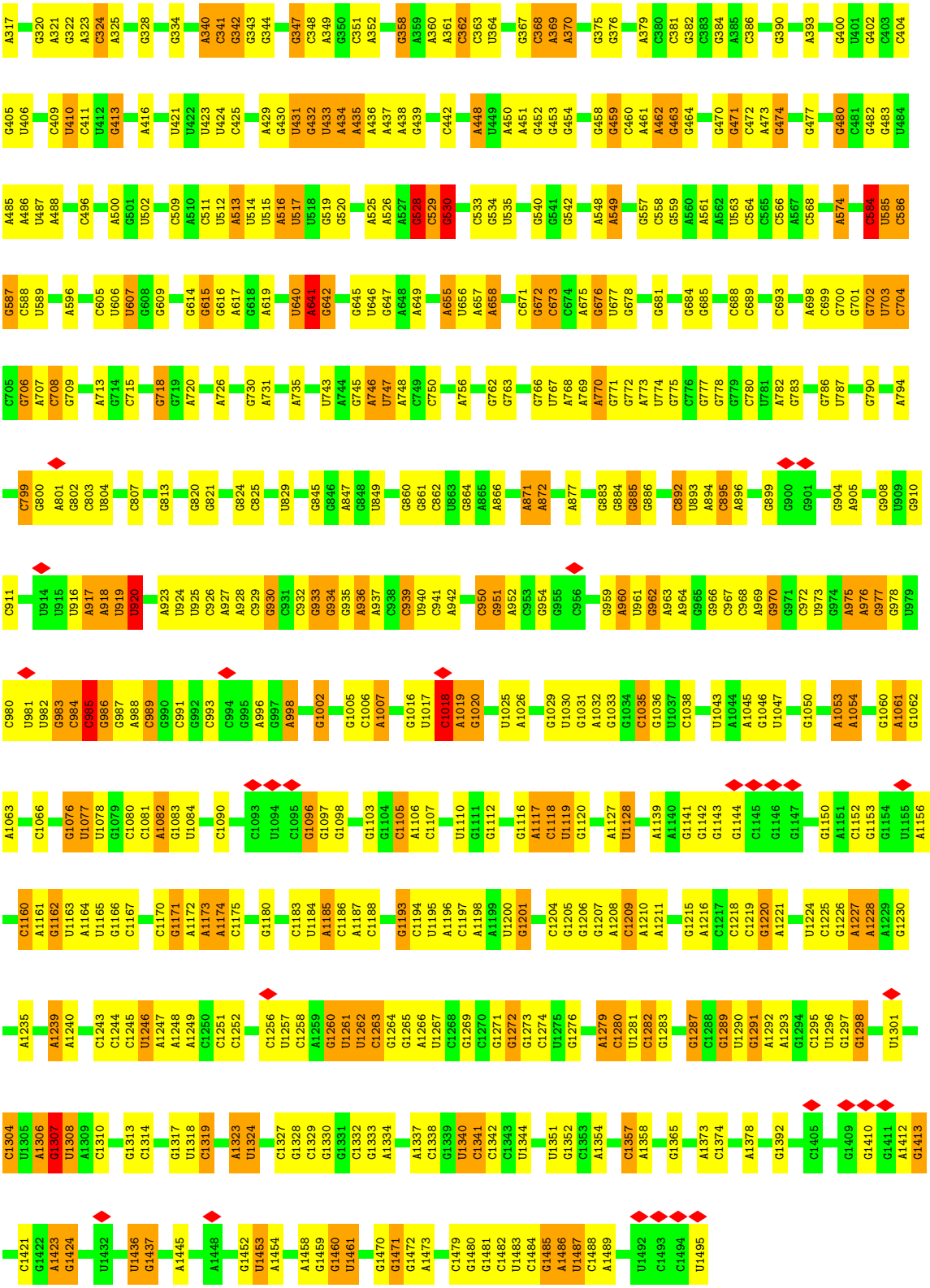




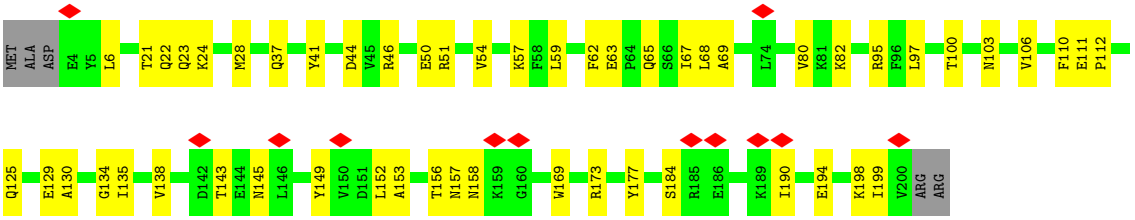
• Molecule 5: 16S rRNA

Chain BA:

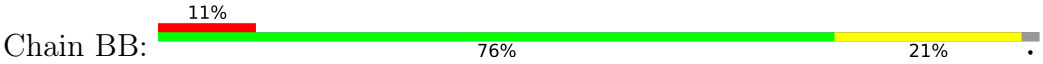


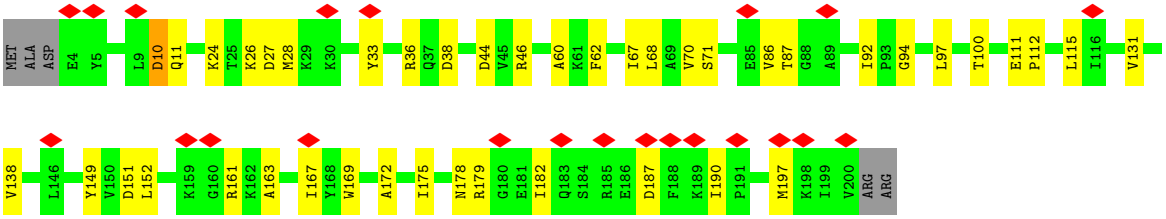


• Molecule 6: Small ribosomal subunit protein uS2

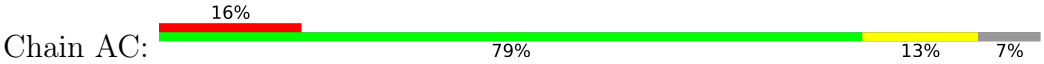


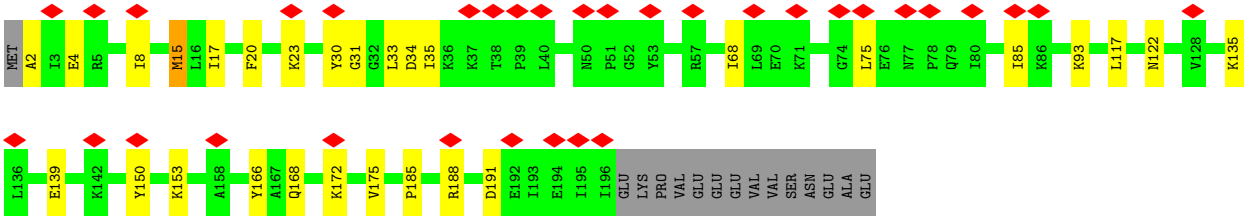
• Molecule 6: Small ribosomal subunit protein uS2



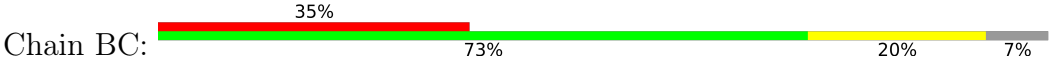


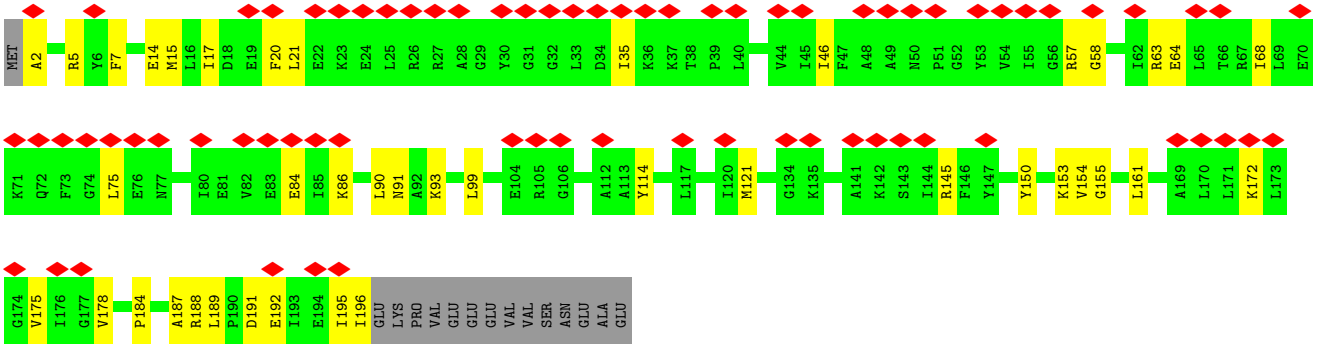
• Molecule 7: Small ribosomal subunit protein uS3



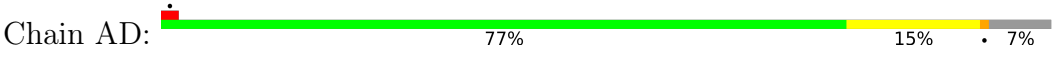


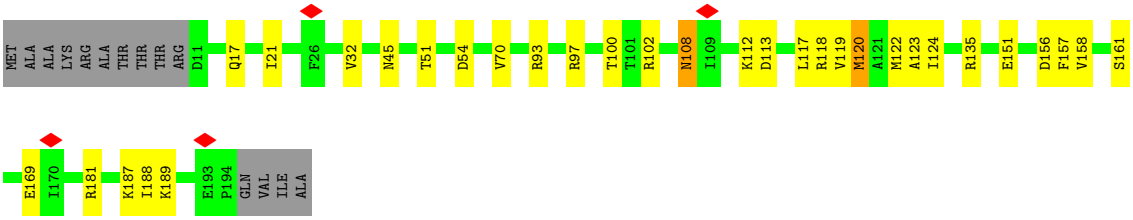
• Molecule 7: Small ribosomal subunit protein uS3





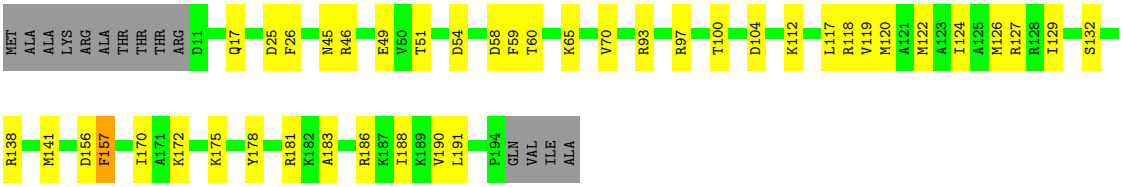
• Molecule 8: Small ribosomal subunit protein eS1





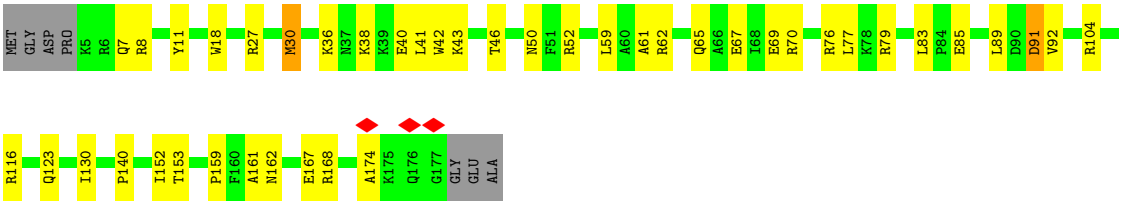
• Molecule 8: Small ribosomal subunit protein eS1

Chain BD:



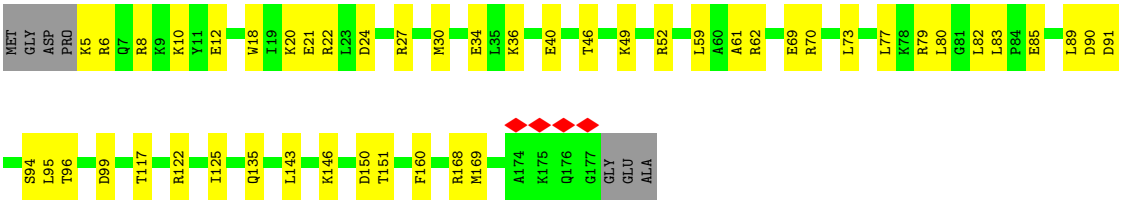
• Molecule 9: Small ribosomal subunit protein uS4

Chain AE:



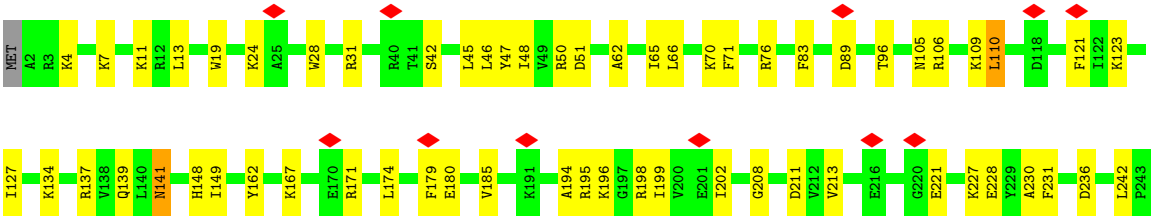
• Molecule 9: Small ribosomal subunit protein uS4

Chain BE:



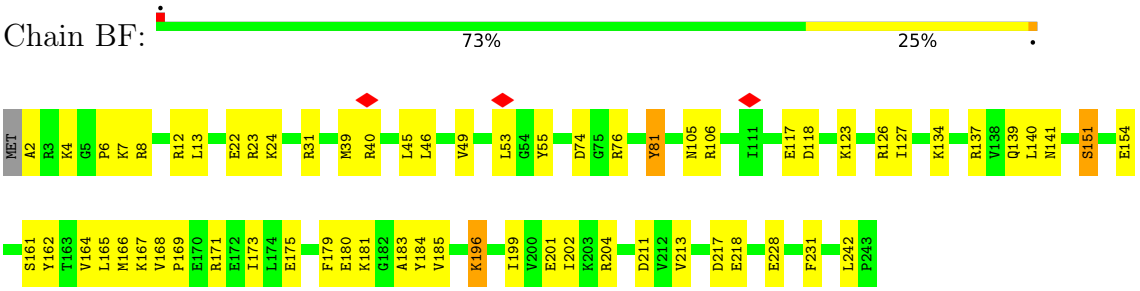
• Molecule 10: Small ribosomal subunit protein eS4

Chain AF:



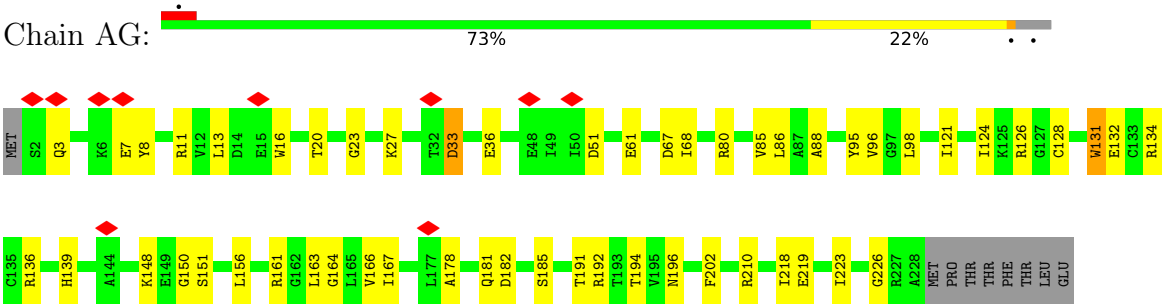
• Molecule 10: Small ribosomal subunit protein eS4

Chain BF:



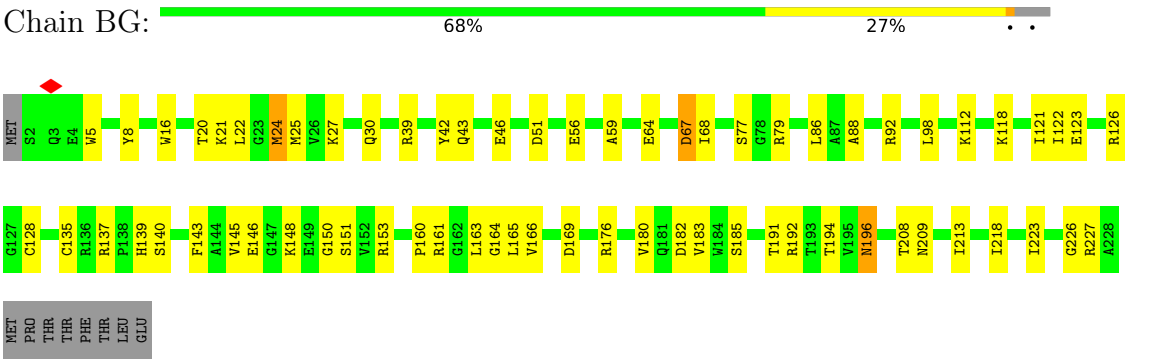
• Molecule 11: Small ribosomal subunit protein uS5

Chain AG:



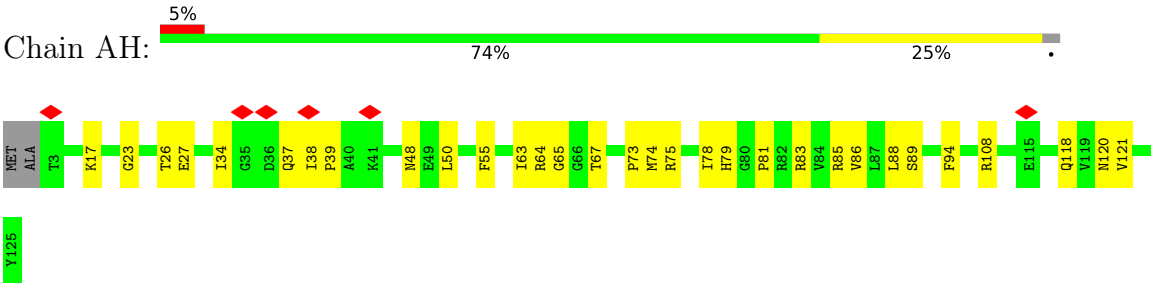
• Molecule 11: Small ribosomal subunit protein uS5

Chain BG:



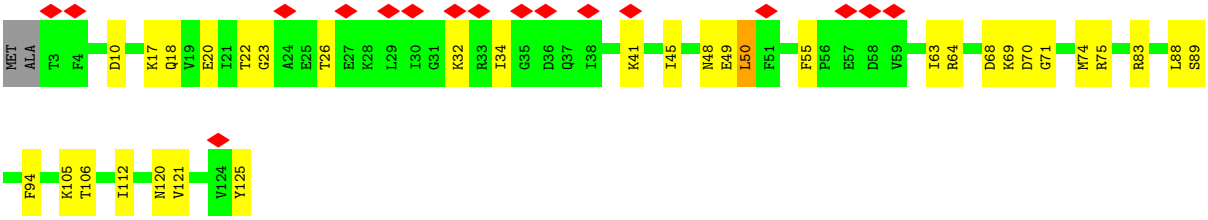
• Molecule 12: Small ribosomal subunit protein eS6

Chain AH:

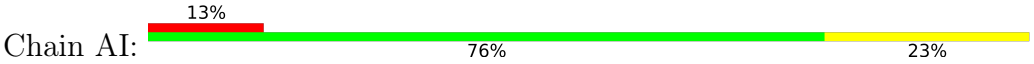


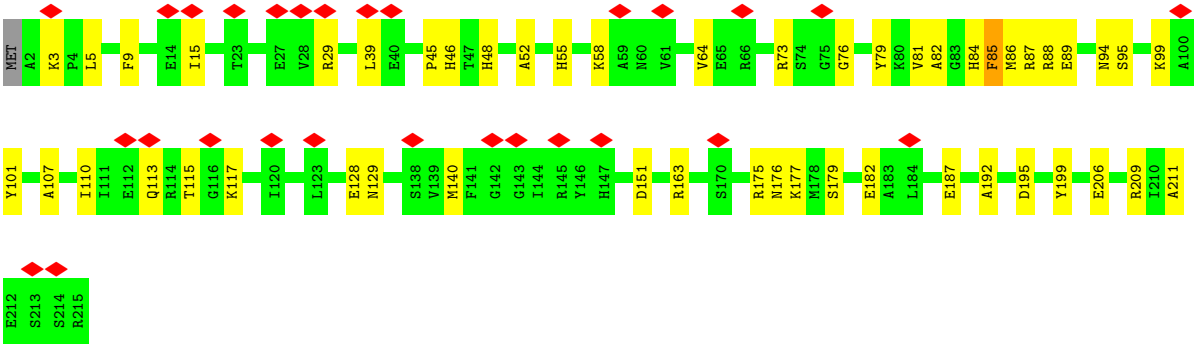
• Molecule 12: Small ribosomal subunit protein eS6

Chain BH:

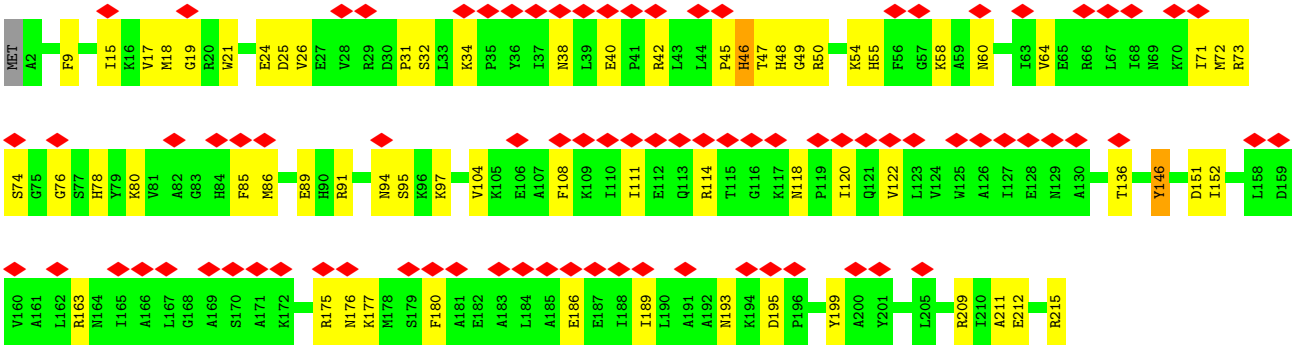


• Molecule 13: Small ribosomal subunit protein uS7

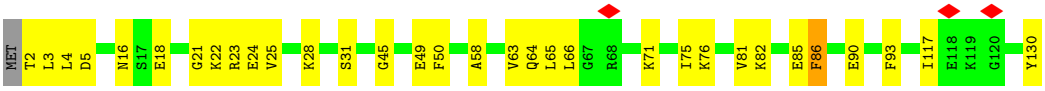




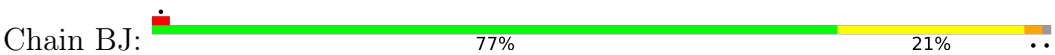
• Molecule 13: Small ribosomal subunit protein uS7

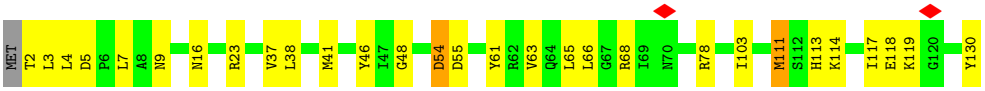


• Molecule 14: Small ribosomal subunit protein uS8

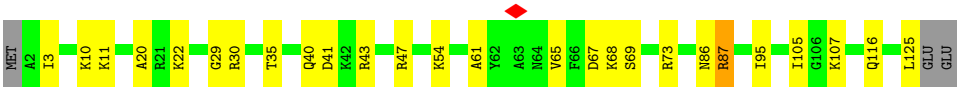


• Molecule 14: Small ribosomal subunit protein uS8



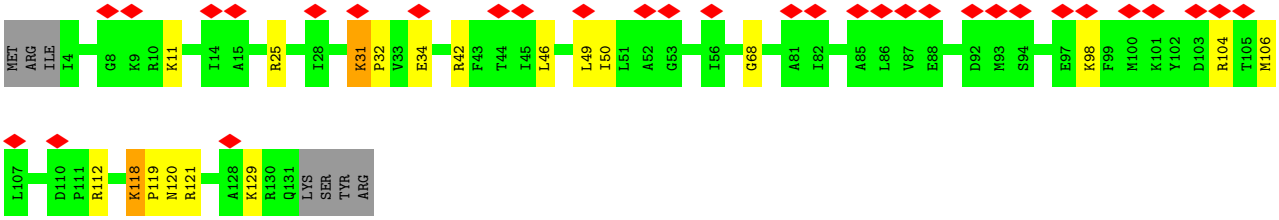


• Molecule 15: Small ribosomal subunit protein eS8

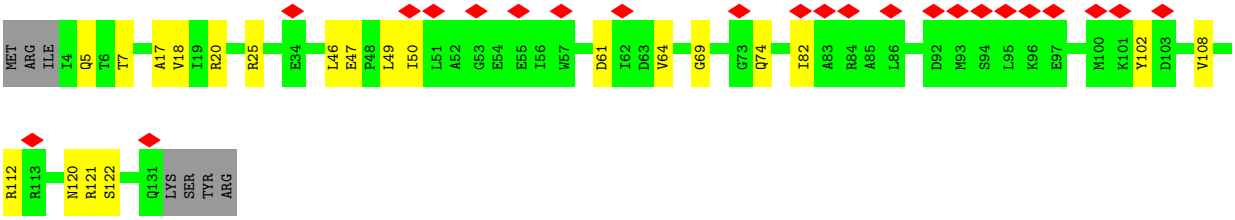


• Molecule 15: Small ribosomal subunit protein eS8

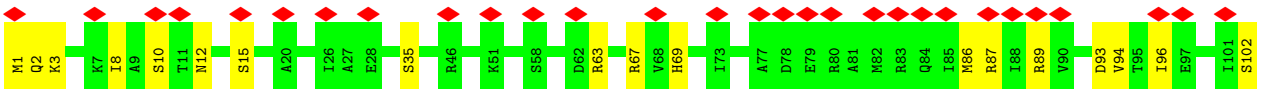
• Molecule 16: Small ribosomal subunit protein uS9



• Molecule 16: Small ribosomal subunit protein uS9

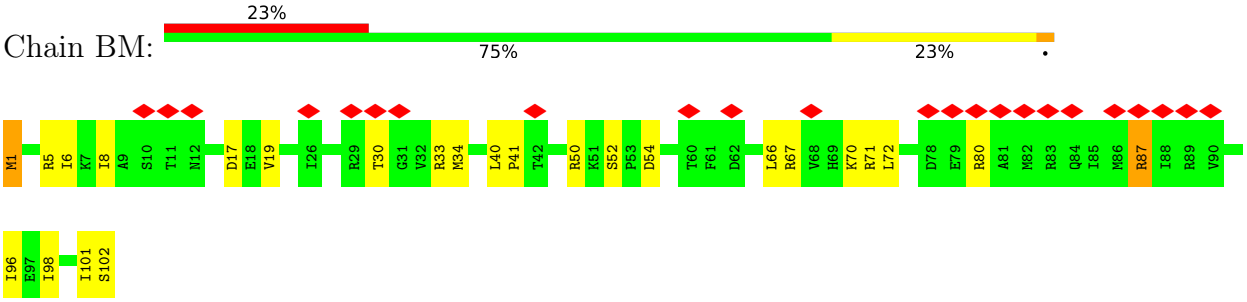


• Molecule 17: Small ribosomal subunit protein uS10



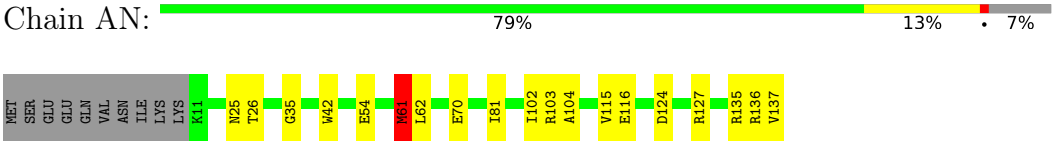
• Molecule 17: Small ribosomal subunit protein uS10

Chain BM:



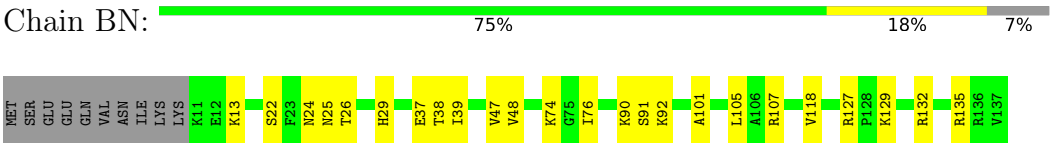
• Molecule 18: Small ribosomal subunit protein uS11

Chain AN:



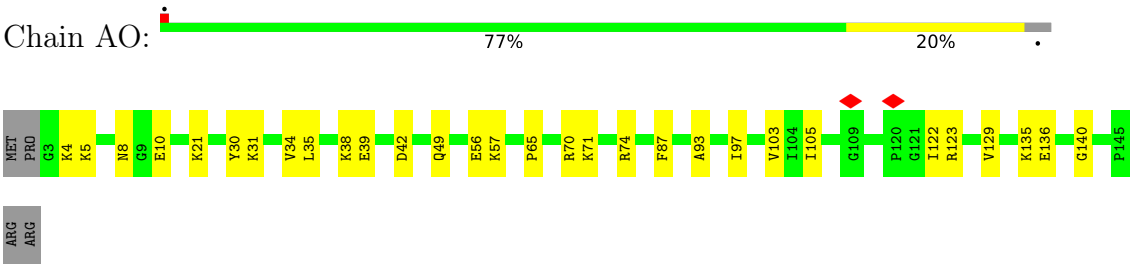
• Molecule 18: Small ribosomal subunit protein uS11

Chain BN:



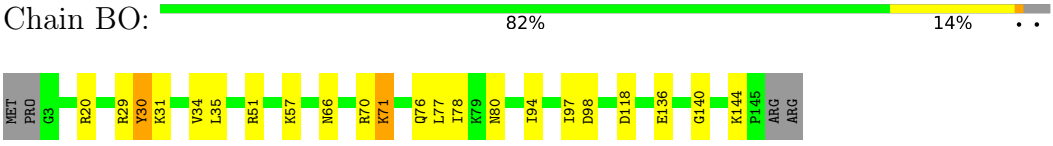
• Molecule 19: Small ribosomal subunit protein uS12

Chain AO:



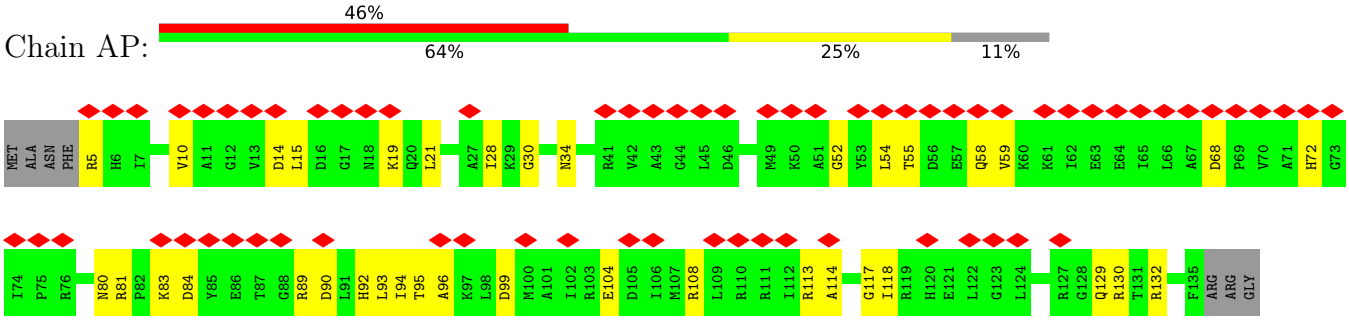
• Molecule 19: Small ribosomal subunit protein uS12

Chain BO:



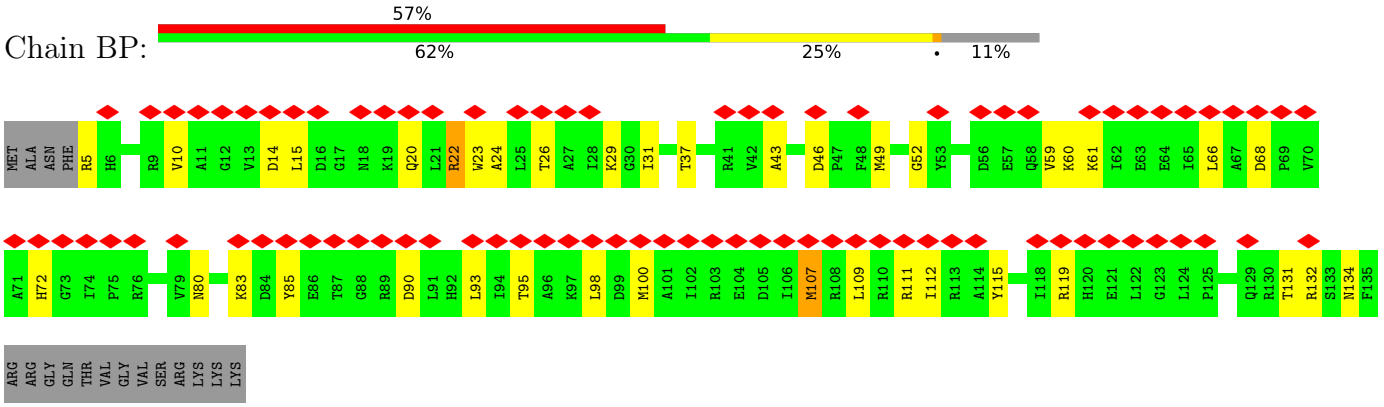
• Molecule 20: Small ribosomal subunit protein uS13

Chain AP:



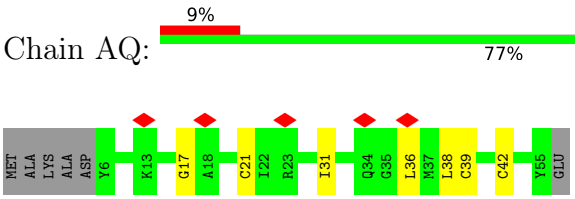
• Molecule 20: Small ribosomal subunit protein uS13

Chain BP:



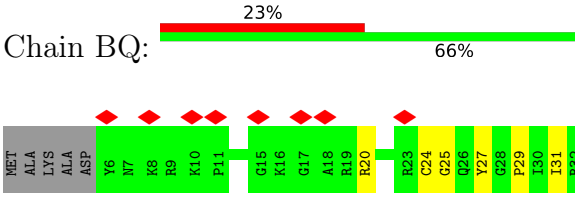
• Molecule 21: Small ribosomal subunit protein uS14

Chain AQ:



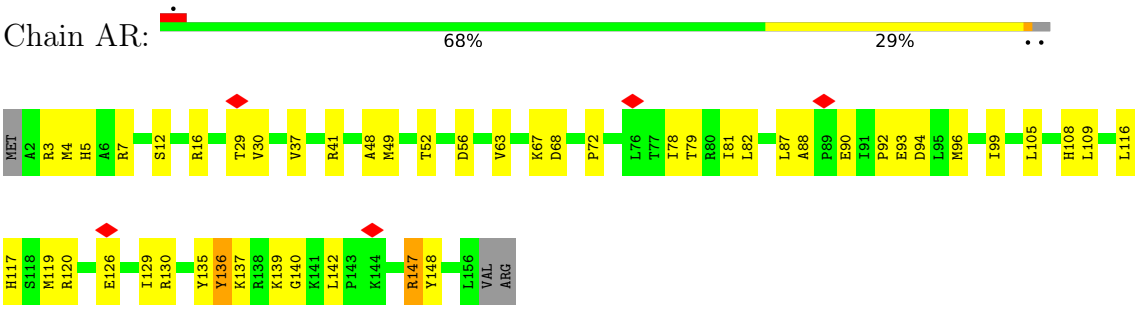
• Molecule 21: Small ribosomal subunit protein uS14

Chain BQ:



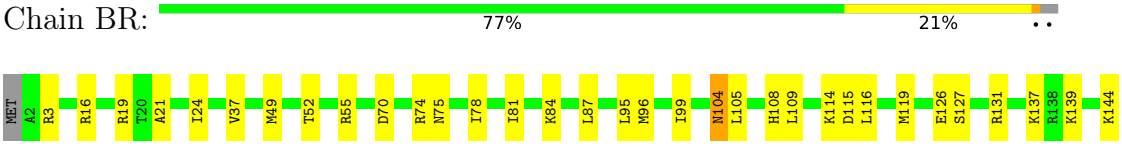
• Molecule 22: Small ribosomal subunit protein uS15

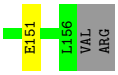
Chain AR:



• Molecule 22: Small ribosomal subunit protein uS15

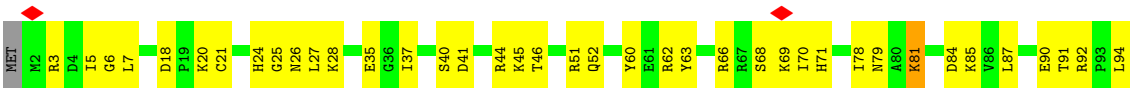
Chain BR:





• Molecule 23: Small ribosomal subunit protein uS17

Chain AS:

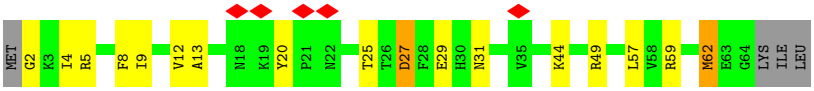


• Molecule 23: Small ribosomal subunit protein uS17

Chain BS:

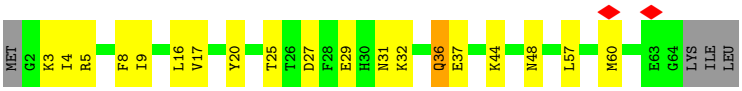
• Molecule 24: Small ribosomal subunit protein eS17

Chain AT:



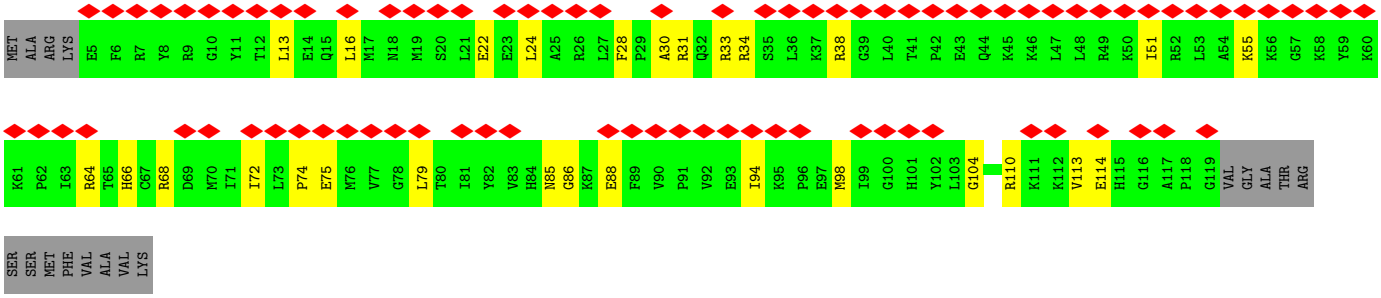
• Molecule 24: Small ribosomal subunit protein eS17

Chain BT:



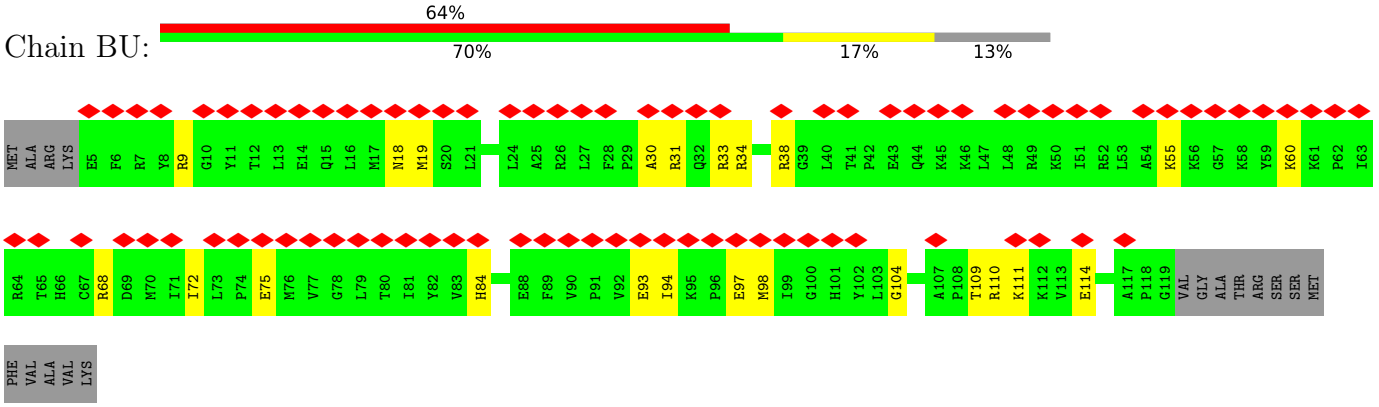
• Molecule 25: Small ribosomal subunit protein uS19

Chain AU:



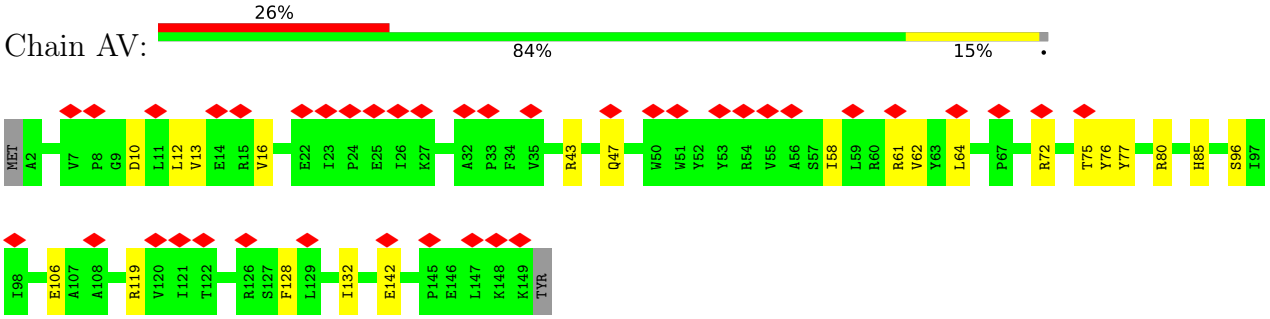
• Molecule 25: Small ribosomal subunit protein uS19

Chain BU:



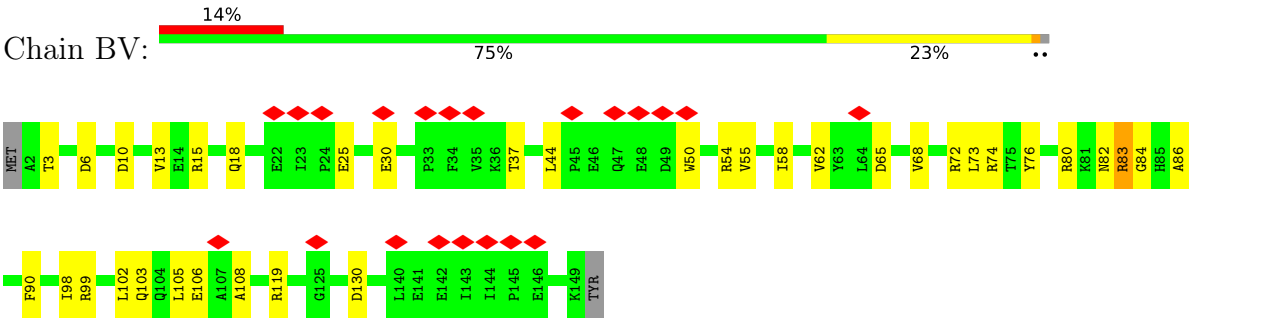
• Molecule 26: Small ribosomal subunit protein eS19

Chain AV:



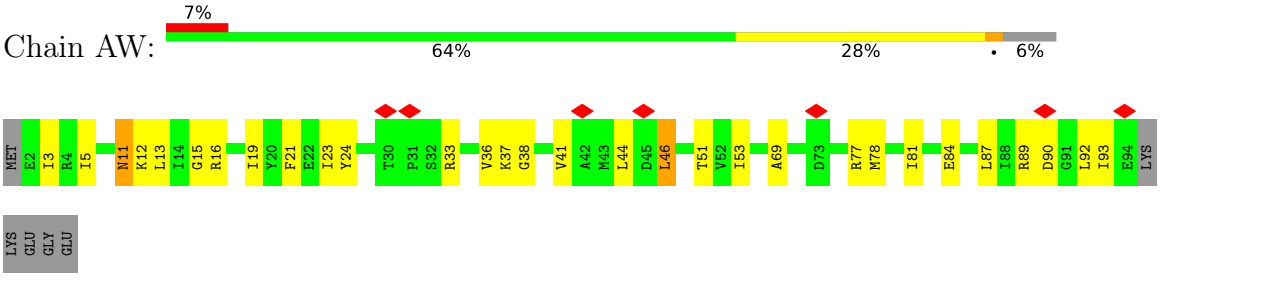
• Molecule 26: Small ribosomal subunit protein eS19

Chain BV:



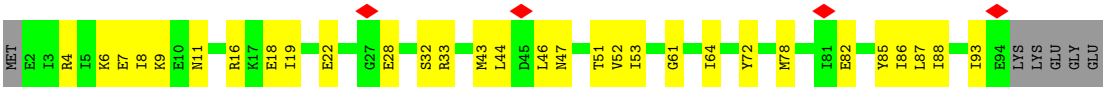
• Molecule 27: Small ribosomal subunit protein eS24

Chain AW:

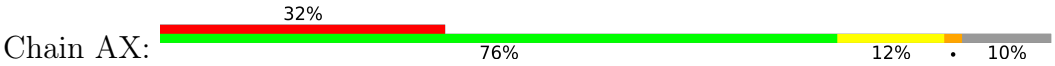


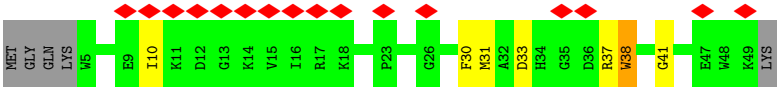
• Molecule 27: Small ribosomal subunit protein eS24

Chain BW:

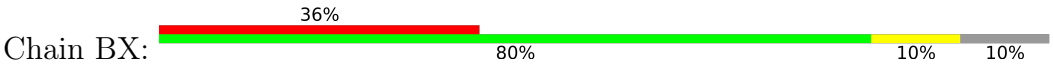


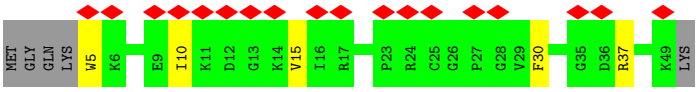
• Molecule 28: Small ribosomal subunit protein eS31



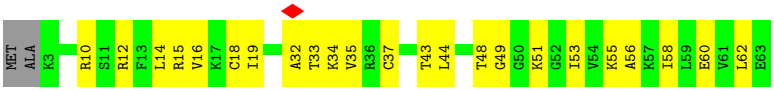


• Molecule 28: Small ribosomal subunit protein eS31

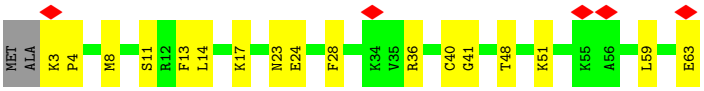




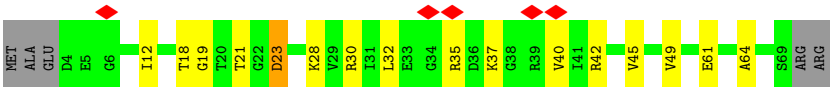
• Molecule 29: Small ribosomal subunit protein eS27



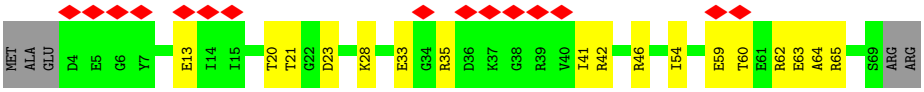
• Molecule 29: Small ribosomal subunit protein eS27



• Molecule 30: Small ribosomal subunit protein eS28



• Molecule 30: Small ribosomal subunit protein eS28



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	63890	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	19.620	Depositor
Minimum map value	-7.838	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.848	Depositor
Recommended contour level	3	Depositor
Map size (Å)	480.384, 480.384, 480.384	wwPDB
Map dimensions	576, 576, 576	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.834, 0.834, 0.834	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A1	0.38	0/485	0.62	0/656
1	B1	0.35	0/485	0.60	0/656
2	A2	0.50	0/341	0.89	0/440
2	B2	0.42	0/341	0.87	0/440
3	A3	0.37	0/2407	0.59	0/3233
3	A4	0.38	0/2353	0.59	0/3161
3	B3	0.36	0/2414	0.58	0/3244
3	B4	0.37	0/2333	0.61	0/3136
4	A5	0.30	0/951	0.57	0/1281
4	B5	0.28	0/951	0.52	0/1281
5	AA	0.63	0/35966	0.98	34/56138 (0.1%)
5	BA	0.63	0/35966	0.96	47/56138 (0.1%)
6	AB	0.33	0/1610	0.61	0/2177
6	BB	0.32	0/1610	0.61	1/2177 (0.0%)
7	AC	0.29	0/1554	0.65	1/2087 (0.0%)
7	BC	0.30	0/1554	0.62	0/2087
8	AD	0.35	0/1537	0.64	0/2060
8	BD	0.35	0/1537	0.61	0/2060
9	AE	0.32	0/1478	0.69	1/1980 (0.1%)
9	BE	0.32	0/1478	0.64	0/1980
10	AF	0.34	0/2030	0.67	2/2739 (0.1%)
10	BF	0.33	0/2030	0.62	1/2739 (0.0%)
11	AG	0.35	0/1824	0.64	0/2457
11	BG	0.34	0/1824	0.65	1/2457 (0.0%)
12	AH	0.31	0/986	0.61	0/1320
12	BH	0.31	0/986	0.61	0/1320
13	AI	0.30	0/1765	0.63	0/2371
13	BI	0.32	0/1765	0.64	0/2371
14	AJ	0.34	0/1049	0.66	1/1408 (0.1%)
14	BJ	0.40	0/1049	0.73	1/1408 (0.1%)
15	AK	0.31	0/986	0.67	0/1315
15	BK	0.32	0/986	0.67	0/1315
16	AL	0.30	0/1021	0.71	0/1369
16	BL	0.28	0/1021	0.65	0/1369

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	AM	0.28	0/830	0.69	0/1113
17	BM	0.30	0/830	0.70	0/1113
18	AN	0.34	0/972	0.69	1/1309 (0.1%)
18	BN	0.36	0/972	0.68	0/1309
19	AO	0.37	0/1134	0.66	0/1508
19	BO	0.34	0/1134	0.65	0/1508
20	AP	0.29	0/1070	0.69	1/1440 (0.1%)
20	BP	0.32	0/1070	0.69	0/1440
21	AQ	0.31	0/426	0.75	0/562
21	BQ	0.34	0/426	0.83	1/562 (0.2%)
22	AR	0.34	0/1311	0.65	0/1763
22	BR	0.35	0/1311	0.69	1/1763 (0.1%)
23	AS	0.35	0/925	0.63	0/1249
23	BS	0.38	0/925	0.61	0/1249
24	AT	0.33	0/528	0.70	1/701 (0.1%)
24	BT	0.30	0/528	0.65	0/701
25	AU	0.29	0/968	0.67	0/1293
25	BU	0.31	0/968	0.66	0/1293
26	AV	0.29	0/1238	0.59	0/1668
26	BV	0.28	0/1238	0.58	0/1668
27	AW	0.33	0/790	0.66	0/1061
27	BW	0.34	0/790	0.64	0/1061
28	AX	0.29	0/381	0.59	0/509
28	BX	0.28	0/381	0.62	0/509
29	AY	0.32	0/472	0.58	0/634
29	BY	0.32	0/472	0.63	0/634
30	AZ	0.30	0/525	0.69	0/703
30	BZ	0.28	0/525	0.70	0/703
All	All	0.51	0/139813	0.84	95/203396 (0.0%)

There are no bond length outliers.

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	AA	71	C	N3-C2-O2	-10.46	114.58	121.90
5	AA	823	A	O5'-P-OP1	-9.15	97.47	105.70
14	BJ	54	ASP	CB-CG-OD1	8.27	125.75	118.30
5	BA	1471	G	N3-C4-N9	-8.02	121.19	126.00
5	BA	18	C	N3-C2-O2	-7.85	116.41	121.90
9	AE	91	ASP	CB-CG-OD1	7.62	125.16	118.30
5	AA	708	C	C2-N1-C1'	6.92	126.41	118.80
5	BA	530	G	N3-C4-C5	6.71	131.96	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	BA	985	C	N3-C2-O2	-6.63	117.26	121.90
5	BA	530	G	N3-C4-N9	-6.57	122.06	126.00
5	AA	71	C	C6-N1-C2	-6.51	117.69	120.30
10	AF	51	ASP	CB-CG-OD1	6.51	124.16	118.30
5	BA	72	C	N3-C2-O2	-6.41	117.41	121.90
5	BA	433	U	C2-N1-C1'	6.35	125.32	117.70
20	AP	99	ASP	CB-CG-OD1	6.31	123.98	118.30
11	BG	67	ASP	CB-CG-OD1	6.28	123.95	118.30
21	BQ	29	PRO	N-CA-CB	-6.20	95.78	102.60
5	BA	106	A	N1-C6-N6	-6.19	114.89	118.60
5	BA	99	C	C6-N1-C2	-6.17	117.83	120.30
5	AA	528	G	C8-N9-C4	-6.11	103.96	106.40
5	BA	718	G	N3-C2-N2	-6.05	115.67	119.90
5	BA	1471	G	N3-C4-C5	6.04	131.62	128.60
10	BF	118	ASP	CB-CG-OD1	6.04	123.74	118.30
5	AA	1364	C	N1-C2-O2	6.04	122.52	118.90
5	BA	235	G	N1-C2-N2	-5.99	110.81	116.20
6	BB	10	ASP	CB-CG-OD1	5.97	123.67	118.30
5	AA	1478	A	N7-C8-N9	5.88	116.74	113.80
10	AF	236	ASP	CB-CG-OD1	5.87	123.58	118.30
5	AA	530	G	N3-C4-N9	-5.86	122.49	126.00
5	BA	718	G	N3-C4-C5	5.85	131.52	128.60
5	AA	71	C	N1-C2-O2	5.77	122.36	118.90
5	BA	1304	C	C2-N1-C1'	5.75	125.12	118.80
5	BA	718	G	N3-C4-N9	-5.74	122.56	126.00
5	AA	564	C	N3-C2-O2	-5.73	117.89	121.90
24	AT	27	ASP	CB-CG-OD1	5.70	123.43	118.30
5	BA	235	G	N3-C2-N2	5.68	123.87	119.90
5	BA	139	C	N3-C4-C5	5.67	124.17	121.90
5	AA	932	C	N3-C2-O2	-5.65	117.94	121.90
5	AA	56	A	P-O3'-C3'	5.63	126.45	119.70
5	BA	112	G	C2-N3-C4	-5.60	109.10	111.90
5	AA	1364	C	N3-C2-O2	-5.57	118.00	121.90
5	BA	920	U	N1-C2-N3	5.54	118.23	114.90
5	AA	583	G	N3-C4-N9	-5.53	122.68	126.00
5	BA	7	G	N3-C4-N9	-5.46	122.72	126.00
5	BA	1304	C	N3-C4-N4	5.45	121.81	118.00
5	BA	708	C	C2-N1-C1'	5.43	124.78	118.80
5	BA	516	A	C4-N9-C1'	5.43	136.07	126.30
5	AA	871	A	P-O3'-C3'	5.43	126.21	119.70
22	BR	115	ASP	CB-CG-OD1	5.42	123.18	118.30
5	BA	1018	C	C6-N1-C2	-5.40	118.14	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	BA	1201	G	C4-N9-C1'	5.39	133.50	126.50
5	AA	516	A	C4-N9-C1'	5.37	135.97	126.30
5	BA	1035	C	C6-N1-C2	-5.35	118.16	120.30
14	AJ	5	ASP	CB-CG-OD2	5.35	123.11	118.30
5	AA	1245	C	P-O3'-C3'	5.33	126.10	119.70
5	AA	1483	U	C5-C6-N1	5.33	125.36	122.70
5	BA	1453	U	P-O3'-C3'	5.32	126.09	119.70
5	AA	984	C	C6-N1-C2	-5.32	118.17	120.30
5	BA	106	A	C4-C5-C6	-5.32	114.34	117.00
5	BA	1471	G	C8-N9-C1'	5.32	133.91	127.00
5	BA	614	G	N7-C8-N9	5.31	115.76	113.10
5	BA	448	A	N1-C6-N6	-5.31	115.42	118.60
5	AA	1161	A	P-O3'-C3'	5.30	126.06	119.70
5	BA	871	A	P-O3'-C3'	5.30	126.06	119.70
5	BA	516	A	C8-N9-C1'	-5.29	118.18	127.70
5	BA	528	G	P-O3'-C3'	5.28	126.04	119.70
5	AA	388	G	N3-C4-N9	5.28	129.17	126.00
5	BA	112	G	C6-C5-N7	-5.27	127.24	130.40
18	AN	61	MET	CA-CB-CG	5.25	122.23	113.30
5	BA	7	G	C5-C6-O6	5.25	131.75	128.60
5	BA	235	G	N3-C4-N9	5.22	129.13	126.00
5	AA	178	C	N1-C2-O2	5.20	122.02	118.90
5	AA	229	G	N9-C4-C5	-5.20	103.32	105.40
5	AA	386	C	C5-C6-N1	5.20	123.60	121.00
5	AA	1345	G	N3-C4-N9	-5.18	122.89	126.00
5	AA	1484	C	N3-C2-O2	-5.15	118.30	121.90
5	BA	1352	G	C4-N9-C1'	5.15	133.19	126.50
5	BA	235	G	C6-C5-N7	-5.14	127.31	130.40
5	AA	587	G	C8-N9-C1'	-5.14	120.32	127.00
5	AA	871	A	OP2-P-O3'	5.13	116.50	105.20
5	AA	229	G	C4-C5-N7	5.12	112.85	110.80
5	AA	1288	C	N3-C2-O2	-5.12	118.32	121.90
5	BA	584	C	C6-N1-C2	-5.09	118.27	120.30
5	BA	42	G	P-O3'-C3'	5.08	125.79	119.70
5	AA	516	A	C8-N9-C1'	-5.07	118.58	127.70
5	AA	178	C	C2-N1-C1'	5.07	124.37	118.80
5	AA	932	C	N1-C2-O2	5.06	121.93	118.90
5	BA	985	C	N1-C2-O2	5.04	121.92	118.90
5	BA	1307	G	C8-N9-C4	-5.03	104.39	106.40
7	AC	15	MET	CA-CB-CG	5.03	121.84	113.30
5	BA	1452	G	N1-C6-O6	-5.03	116.88	119.90
5	BA	641	A	C8-N9-C4	-5.01	103.80	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	BA	106	A	C6-C5-N7	5.01	135.81	132.30
5	BA	1289	G	C4-C5-N7	5.01	112.80	110.80
5	AA	718	G	C2-N3-C4	-5.00	109.40	111.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A1	471	0	455	14	0
1	B1	471	0	457	13	0
2	A2	335	0	396	16	0
2	B2	335	0	396	12	0
3	A3	2375	0	2527	55	0
3	A4	2321	0	2470	44	0
3	B3	2381	0	2533	45	0
3	B4	2301	0	2444	38	0
4	A5	939	0	994	16	0
4	B5	939	0	994	20	0
5	AA	32135	0	16231	455	0
5	BA	32135	0	16231	430	0
6	AB	1579	0	1638	34	0
6	BB	1579	0	1638	28	0
7	AC	1532	0	1622	18	0
7	BC	1532	0	1622	28	0
8	AD	1511	0	1595	21	0
8	BD	1511	0	1595	26	0
9	AE	1455	0	1531	28	0
9	BE	1455	0	1531	38	0
10	AF	1981	0	2051	41	0
10	BF	1981	0	2051	42	0
11	AG	1794	0	1850	37	0
11	BG	1794	0	1850	48	0
12	AH	971	0	1027	25	0
12	BH	971	0	1027	23	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	AI	1728	0	1775	32	0
13	BI	1728	0	1775	47	0
14	AJ	1028	0	1065	22	0
14	BJ	1028	0	1065	20	0
15	AK	977	0	1064	20	0
15	BK	977	0	1064	15	0
16	AL	1006	0	1052	15	0
16	BL	1006	0	1052	19	0
17	AM	822	0	870	9	0
17	BM	822	0	870	16	0
18	AN	954	0	981	15	0
18	BN	954	0	981	18	0
19	AO	1118	0	1214	28	0
19	BO	1118	0	1214	15	0
20	AP	1052	0	1094	25	0
20	BP	1052	0	1094	28	0
21	AQ	417	0	445	6	0
21	BQ	417	0	445	9	0
22	AR	1283	0	1358	37	0
22	BR	1283	0	1358	32	0
23	AS	903	0	922	37	0
23	BS	903	0	922	24	0
24	AT	522	0	557	13	0
24	BT	522	0	557	15	0
25	AU	948	0	1007	27	0
25	BU	948	0	1007	20	0
26	AV	1209	0	1254	18	0
26	BV	1209	0	1254	31	0
27	AW	774	0	794	18	0
27	BW	774	0	794	20	0
28	AX	369	0	361	8	0
28	BX	369	0	361	7	0
29	AY	465	0	507	18	0
29	BY	465	0	507	9	0
30	AZ	523	0	551	9	0
30	BZ	523	0	551	12	0
All	All	130980	0	102498	1868	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 8.

All (1868) 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)
5:BA:777:G:HO2'	14:BJ:2:THR:N	1.48	1.11
5:BA:473:A:N6	5:BA:482:G:C2	2.19	1.11
5:BA:16:G:H21	5:BA:872:A:H62	1.12	0.97
5:AA:998:A:H61	5:AA:1173:A:H61	1.17	0.91
5:BA:106:A:H62	5:BA:235:G:N2	1.67	0.91
5:AA:983:G:O2'	5:AA:984:C:O4'	1.89	0.89
5:AA:23:G:O2'	5:AA:292:U:OP1	1.94	0.85
5:AA:619:A:N7	5:AA:678:G:O6	2.08	0.85
13:BI:54:LYS:O	13:BI:58:LYS:NZ	2.10	0.84
5:BA:1365:G:O2'	5:BA:1473:A:O2'	1.95	0.84
10:BF:126:ARG:NH1	10:BF:228:GLU:O	2.10	0.84
5:AA:711:U:OP1	22:AR:7:ARG:NH2	2.12	0.83
5:AA:1460:G:O2'	5:AA:1461:U:OP2	1.96	0.83
5:AA:1392:G:O2'	5:AA:1423:A:N6	2.11	0.83
5:BA:106:A:N6	5:BA:235:G:H21	1.77	0.83
5:AA:5:C:OP2	11:AG:191:THR:OG1	1.96	0.83
5:AA:63:G:O2'	5:AA:156:A:O2'	1.96	0.83
5:AA:136:A:N7	5:AA:155:U:O2	2.12	0.83
5:AA:615:G:O6	5:AA:698:A:N1	2.12	0.83
5:AA:904:G:N2	5:AA:1294:G:O2'	2.11	0.82
5:AA:486:A:O2'	5:AA:488:A:OP2	1.97	0.82
5:BA:1351:U:O2'	5:BA:1487:U:OP1	1.96	0.82
3:A3:86:LEU:HD11	3:A3:92:LEU:HD12	1.62	0.82
5:AA:616:G:O2'	5:AA:790:G:OP1	1.97	0.82
5:BA:262:G:O2'	5:BA:264:C:OP2	1.95	0.82
5:BA:1296:U:OP2	13:BI:175:ARG:NH1	2.13	0.82
5:BA:566:C:O2'	9:BE:69:GLU:OE1	1.97	0.81
5:BA:1280:C:N4	25:BU:68:ARG:O	2.11	0.81
5:AA:497:C:OP1	9:AE:27:ARG:NH2	2.14	0.81
5:AA:1193:G:N2	5:AA:1324:U:O2	2.12	0.81
5:BA:156:A:O2'	5:BA:157:A:O4'	1.98	0.81
5:BA:671:C:O2'	5:BA:688:C:O4'	1.98	0.81
5:AA:247:G:N2	5:AA:249:U:O4	2.13	0.80
5:AA:1120:G:O6	5:AA:1142:G:N2	2.15	0.80
8:AD:45:ASN:N	8:AD:70:VAL:O	2.14	0.80
5:BA:101:G:N2	5:BA:309:A:O2'	2.14	0.80
5:BA:1412:A:O2'	12:BH:75:ARG:NH2	2.15	0.80
3:B4:68:THR:OG1	3:B4:73:LYS:NZ	2.14	0.80
2:A2:15:ARG:NE	5:AA:1465:C:OP2	2.15	0.80
5:AA:946:G:N2	5:AA:974:G:O6	2.15	0.80
5:AA:883:G:O2'	5:AA:885:G:OP1	1.98	0.80
23:BS:32:ARG:N	23:BS:90:GLU:OE1	2.15	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BA:780:C:O2	14:BJ:16:ASN:ND2	2.15	0.79
5:BA:885:G:O2'	5:BA:1458:A:N7	2.15	0.79
5:BA:352:A:N3	5:BA:364:U:O2'	2.14	0.79
5:BA:984:C:O2'	28:BX:30:PHE:O	1.97	0.79
20:AP:104:GLU:OE2	20:AP:108:ARG:NH1	2.15	0.79
5:AA:123:U:OP1	10:AF:76:ARG:NH1	2.16	0.79
5:AA:342:G:O2'	12:AH:83:ARG:NH1	2.15	0.79
5:AA:606:U:O2'	5:AA:607:U:O2	2.01	0.79
5:BA:586:C:O2	5:BA:587:G:N2	2.15	0.79
20:BP:23:TRP:O	20:BP:26:THR:OG1	1.99	0.79
5:BA:1269:G:N2	20:BP:80:ASN:O	2.15	0.79
5:AA:655:A:O2'	5:AA:656:U:OP2	2.01	0.79
5:AA:1283:G:O6	25:AU:31:ARG:NH1	2.16	0.79
5:BA:313:G:N2	5:BA:1424:G:OP1	2.16	0.79
5:BA:960:A:N6	5:BA:989:C:OP2	2.15	0.79
5:BA:886:G:O2'	5:BA:1488:C:O4'	2.01	0.79
5:AA:1197:C:O2'	5:AA:1260:G:N2	2.14	0.78
5:BA:1209:C:O2'	16:BL:69:GLY:O	1.99	0.78
3:A3:50:LYS:O	3:A3:53:THR:OG1	2.01	0.78
5:AA:1047:U:OP1	5:AA:1060:G:N2	2.15	0.78
5:BA:615:G:O6	5:BA:698:A:N1	2.16	0.78
5:BA:1193:G:N2	5:BA:1324:U:O2	2.13	0.78
5:AA:671:C:O2'	5:AA:688:C:O4'	2.00	0.78
5:AA:311:A:OP2	15:AK:22:LYS:NZ	2.16	0.78
5:AA:1194:C:O2'	26:AV:85:HIS:O	2.01	0.78
5:AA:1288:C:OP1	20:AP:34:ASN:ND2	2.16	0.78
23:AS:79:ASN:OD1	23:AS:81:LYS:NZ	2.13	0.78
5:BA:534:G:OP1	22:BR:131:ARG:NH1	2.17	0.78
9:BE:52:ARG:NH2	11:BG:161:ARG:O	2.17	0.78
5:AA:201:G:N2	5:AA:202:G:O6	2.17	0.78
5:AA:261:G:N2	5:AA:263:C:OP1	2.16	0.78
5:BA:23:G:O2'	5:BA:292:U:OP1	2.01	0.78
5:BA:106:A:N6	5:BA:235:G:N2	2.31	0.77
22:BR:74:ARG:NH2	22:BR:75:ASN:O	2.16	0.77
5:BA:19:G:O2'	5:BA:477:G:N3	2.17	0.77
5:BA:1084:U:O2	5:BA:1103:G:N2	2.18	0.77
25:AU:55:LYS:NZ	25:AU:75:GLU:O	2.16	0.77
5:AA:112:G:N2	5:AA:229:G:O6	2.16	0.77
6:BB:111:GLU:OE2	11:BG:20:THR:OG1	2.02	0.77
5:BA:226:G:OP1	10:BF:31:ARG:NH2	2.17	0.77
5:AA:917:A:N1	25:AU:85:ASN:ND2	2.32	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BA:1215:G:OP2	5:BA:1239:A:N6	2.17	0.77
5:AA:1461:U:O2	18:AN:136:ARG:NE	2.14	0.77
5:AA:964:A:N6	5:AA:989:C:O2'	2.18	0.76
5:BA:910:G:N3	5:BA:929:C:O2'	2.18	0.76
5:BA:934:G:N2	5:BA:1317:G:O2'	2.18	0.76
10:BF:151:SER:OG	10:BF:154:GLU:OE2	2.01	0.76
5:BA:473:A:C6	5:BA:482:G:N2	2.53	0.76
22:AR:147:ARG:NH1	22:AR:148:TYR:O	2.18	0.76
3:B3:47:GLU:O	3:B3:104:ARG:NH1	2.17	0.76
5:BA:1153:G:O2'	11:BG:77:SER:O	2.03	0.76
5:AA:897:A:N3	5:AA:1336:U:O2'	2.17	0.76
5:AA:1272:G:OP2	25:AU:30:ALA:N	2.19	0.76
10:BF:6:PRO:O	10:BF:8:ARG:NH1	2.19	0.76
19:BO:57:LYS:NZ	19:BO:97:ILE:O	2.15	0.76
5:AA:180:G:N2	5:AA:183:A:OP2	2.16	0.76
5:BA:369:A:O2'	5:BA:370:A:O5'	2.04	0.76
5:BA:821:G:OP1	11:BG:153:ARG:NH2	2.19	0.76
5:BA:1460:G:O2'	5:BA:1461:U:OP2	2.03	0.76
5:AA:352:A:N3	5:AA:364:U:O2'	2.18	0.76
5:AA:1138:G:N2	5:AA:1141:G:OP2	2.18	0.76
19:BO:70:ARG:NH2	19:BO:118:ASP:OD2	2.18	0.76
5:AA:821:G:N2	5:AA:824:G:OP2	2.19	0.76
5:AA:1412:A:O2'	12:AH:75:ARG:NH2	2.19	0.76
9:AE:159:PRO:O	9:AE:162:ASN:ND2	2.19	0.75
5:BA:1209:C:N4	5:BA:1248:A:OP2	2.19	0.75
2:A2:9:LYS:O	2:A2:13:ARG:NH1	2.18	0.75
5:AA:1477:U:OP1	18:AN:136:ARG:NH2	2.20	0.75
5:BA:362:C:O2	5:BA:390:G:N2	2.19	0.75
5:BA:640:U:O2'	5:BA:641:A:O5'	2.03	0.75
5:BA:1007:A:N6	5:BA:1160:C:O2	2.18	0.75
5:BA:1224:U:OP1	26:BV:119:ARG:NH2	2.18	0.75
5:BA:783:G:OP1	6:BB:26:LYS:NZ	2.15	0.75
5:BA:293:G:N2	5:BA:296:A:OP2	2.20	0.75
25:BU:68:ARG:NH2	25:BU:104:GLY:O	2.19	0.75
5:AA:730:G:N2	5:AA:756:A:OP2	2.20	0.75
2:B2:34:ARG:NE	2:B2:34:ARG:O	2.20	0.75
5:BA:16:G:O2'	5:BA:17:C:O4'	2.04	0.75
24:AT:27:ASP:O	24:AT:31:ASN:ND2	2.19	0.75
5:BA:968:C:N4	5:BA:982:U:O2	2.19	0.75
5:AA:331:C:O2'	5:AA:1393:A:N3	2.19	0.75
5:BA:322:G:OP2	15:BK:47:ARG:NH2	2.20	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AA:836:G:OP2	19:AO:4:LYS:NZ	2.15	0.75
5:BA:432:G:O2'	5:BA:437:A:N6	2.14	0.75
5:BA:1062:G:N2	7:BC:191:ASP:OD2	2.20	0.75
13:BI:136:THR:O	30:BZ:46:ARG:NH2	2.20	0.74
23:BS:50:GLU:OE2	23:BS:52:GLN:NE2	2.20	0.74
5:AA:1275:U:C2	5:AA:1279:A:N6	2.55	0.74
19:AO:34:VAL:HG13	19:AO:35:LEU:HD22	1.67	0.74
20:AP:5:ARG:N	20:AP:52:GLY:O	2.20	0.74
5:BA:1264:G:H21	5:BA:1293:A:H62	1.34	0.74
5:BA:1308:U:O2	5:BA:1334:A:N6	2.12	0.74
5:AA:532:C:O2'	22:AR:120:ARG:NH2	2.20	0.74
5:AA:566:C:O2'	9:AE:69:GLU:OE2	2.02	0.74
5:AA:434:A:OP1	5:AA:435:A:N6	2.20	0.74
5:AA:777:G:HO2'	14:AJ:2:THR:N	1.86	0.74
5:AA:780:C:O2	14:AJ:16:ASN:ND2	2.20	0.74
5:AA:899:G:OP2	13:AI:79:TYR:OH	2.05	0.74
5:BA:5:C:OP2	11:BG:191:THR:OG1	2.04	0.74
5:BA:471:G:N2	19:BO:66:ASN:OD1	2.19	0.74
5:AA:156:A:O2'	5:AA:157:A:O4'	2.05	0.74
5:BA:1063:A:O2'	7:BC:191:ASP:OD1	2.02	0.74
5:AA:27:C:O2'	19:AO:49:GLN:OE1	2.02	0.74
18:AN:25:ASN:ND2	18:AN:54:GLU:OE1	2.21	0.74
5:AA:1307:G:HO2'	5:AA:1333:G:H1	1.31	0.74
26:BV:37:THR:OG1	26:BV:54:ARG:NH2	2.21	0.74
5:BA:473:A:N6	5:BA:482:G:N2	2.36	0.73
6:AB:63:GLU:OE1	6:AB:65:GLN:NE2	2.21	0.73
5:BA:180:G:N2	5:BA:183:A:OP2	2.20	0.73
5:BA:1118:C:OP1	24:BT:48:ASN:ND2	2.21	0.73
2:B2:1:MET:N	5:BA:862:C:OP2	2.21	0.73
5:BA:1262:U:O2'	5:BA:1263:C:OP1	2.06	0.73
12:BH:10:ASP:OD1	12:BH:125:TYR:OH	2.03	0.73
12:BH:23:GLY:O	12:BH:26:THR:OG1	2.05	0.73
5:AA:706:G:O2'	5:AA:707:A:OP2	2.06	0.73
5:BA:463:G:OP1	9:BE:20:LYS:NZ	2.22	0.73
9:BE:90:ASP:OD1	11:BG:161:ARG:NH1	2.21	0.73
5:AA:1116:G:OP2	24:AT:44:LYS:NZ	2.14	0.73
5:AA:1207:G:OP2	26:AV:76:TYR:OH	2.04	0.73
5:AA:846:G:OP2	5:AA:847:A:O2'	2.04	0.73
20:AP:68:ASP:OD1	20:AP:89:ARG:NH2	2.21	0.73
3:A3:50:LYS:NZ	3:A4:188:GLU:O	2.21	0.73
5:BA:703:U:OP1	22:BR:55:ARG:NH1	2.22	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:BI:48:HIS:O	16:BL:112:ARG:NH1	2.22	0.73
3:A3:143:TYR:O	3:A3:146:THR:OG1	2.06	0.73
5:AA:101:G:N2	15:AK:20:ALA:O	2.17	0.72
5:AA:368:C:N4	5:AA:384:G:OP2	2.22	0.72
14:AJ:85:GLU:OE1	14:AJ:85:GLU:N	2.22	0.72
5:BA:824:G:O2'	5:BA:877:A:OP1	2.05	0.72
4:A5:15:LEU:HG	4:A5:78:ILE:HD11	1.71	0.72
5:AA:1183:C:OP2	25:AU:110:ARG:NH2	2.22	0.72
5:BA:151:G:O3'	12:BH:64:ARG:NH1	2.23	0.72
22:AR:67:LYS:NZ	22:AR:68:ASP:O	2.19	0.72
5:AA:262:G:O2'	5:AA:264:C:OP2	2.02	0.72
23:AS:26:ASN:O	23:AS:28:LYS:NZ	2.21	0.72
5:AA:340:A:OP2	5:AA:341:C:N4	2.23	0.72
3:B4:271:SER:OG	3:B4:273:GLU:OE1	2.06	0.72
5:AA:142:G:H21	12:AH:67:THR:HG21	1.54	0.72
16:AL:34:GLU:O	16:AL:42:ARG:NH1	2.23	0.72
12:BH:49:GLU:N	12:BH:49:GLU:OE1	2.22	0.72
11:AG:163:LEU:N	11:AG:182:ASP:OD1	2.23	0.72
17:AM:3:LYS:NZ	17:AM:102:SER:O	2.23	0.72
5:AA:451:A:O4'	5:AA:500:A:N6	2.23	0.72
5:AA:1007:A:O2'	7:AC:139:GLU:OE2	2.08	0.72
5:BA:1083:G:OP1	16:BL:20:ARG:NH1	2.23	0.71
3:A3:134:LEU:O	3:A3:140:ARG:NH1	2.23	0.71
5:AA:5:C:O2'	5:AA:459:G:O3'	2.07	0.71
5:AA:562:A:O3'	10:AF:24:LYS:NZ	2.23	0.71
5:AA:1030:U:O2	11:AG:196:ASN:ND2	2.23	0.71
3:B4:272:GLU:OE1	3:B4:272:GLU:N	2.22	0.71
5:BA:977:G:N2	5:BA:980:C:OP2	2.23	0.71
21:BQ:20:ARG:NH1	21:BQ:25:GLY:O	2.23	0.71
5:BA:777:G:O3'	22:BR:3:ARG:NH2	2.23	0.71
12:BH:17:LYS:NZ	12:BH:50:LEU:O	2.23	0.71
5:BA:5:C:O2'	5:BA:459:G:O3'	2.07	0.71
5:BA:1221:A:O2'	26:BV:72:ARG:NH2	2.23	0.71
5:BA:1225:C:OP2	26:BV:103:GLN:NE2	2.23	0.71
5:AA:46:A:O2'	5:AA:356:G:N2	2.24	0.71
5:AA:176:U:O2'	5:AA:177:A:OP1	2.08	0.71
5:BA:1208:A:O2'	16:BL:74:GLN:OE1	2.05	0.71
5:BA:1019:A:O2'	5:BA:1020:G:OP2	2.07	0.71
5:AA:400:G:N2	5:AA:450:A:N7	2.39	0.71
25:AU:51:ILE:HD11	25:AU:79:LEU:HD13	1.72	0.71
5:AA:1269:G:N2	20:AP:80:ASN:O	2.23	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:BT:27:ASP:O	24:BT:31:ASN:ND2	2.23	0.71
5:AA:433:U:OP2	5:AA:434:A:O2'	2.08	0.71
5:AA:1263:C:OP1	26:AV:43:ARG:NH2	2.24	0.71
22:AR:109:LEU:HD21	22:AR:119:MET:SD	2.31	0.71
3:B4:148:ASN:ND2	3:B4:251:SER:O	2.23	0.71
12:BH:48:ASN:OD1	12:BH:55:PHE:N	2.24	0.70
10:AF:70:LYS:NZ	27:AW:13:LEU:O	2.24	0.70
3:B3:247:ASP:OD2	3:B3:250:LEU:N	2.24	0.70
5:BA:892:C:O2'	5:BA:1304:C:OP2	2.08	0.70
5:BA:960:A:O4'	5:BA:988:A:N6	2.24	0.70
6:BB:36:ARG:NH1	6:BB:38:ASP:OD2	2.22	0.70
8:AD:97:ARG:O	8:AD:100:THR:OG1	2.09	0.70
5:AA:1219:C:O2'	5:AA:1243:C:O2	2.09	0.70
5:BA:176:U:O2'	5:BA:177:A:OP1	2.08	0.70
5:BA:1267:U:O4	5:BA:1291:G:N2	2.19	0.70
5:AA:266:A:O3'	15:AK:87:ARG:NH2	2.25	0.70
5:BA:1080:C:O2'	5:BA:1082:A:OP2	2.06	0.70
5:AA:1260:G:O2'	5:AA:1263:C:N4	2.24	0.70
5:BA:434:A:OP1	5:BA:435:A:N6	2.22	0.70
5:BA:1119:U:OP1	24:BT:3:LYS:NZ	2.25	0.70
6:BB:71:SER:O	6:BB:94:GLY:N	2.23	0.70
5:AA:106:A:O2'	5:AA:308:G:O2'	2.10	0.70
5:AA:242:A:N1	5:AA:274:G:O2'	2.23	0.70
3:A4:168:ARG:NE	3:A4:168:ARG:O	2.25	0.69
8:AD:21:ILE:HD11	8:AD:32:VAL:HB	1.74	0.69
19:AO:136:GLU:O	19:AO:140:GLY:N	2.25	0.69
5:AA:6:G:O6	11:AG:192:ARG:NH2	2.25	0.69
5:AA:1044:A:N7	24:AT:2:GLY:N	2.39	0.69
5:BA:16:G:N2	5:BA:872:A:H62	1.88	0.69
5:BA:528:G:O2'	5:BA:529:C:OP2	2.09	0.69
5:BA:962:G:N2	5:BA:988:A:N7	2.40	0.69
12:AH:74:MET:N	12:AH:74:MET:SD	2.66	0.69
3:B4:287:ILE:O	3:B4:290:SER:OG	2.03	0.69
5:BA:645:G:OP1	18:BN:90:LYS:NZ	2.24	0.69
5:BA:563:U:OP1	10:BF:24:LYS:NZ	2.23	0.69
5:BA:1436:U:O2'	5:BA:1437:G:OP1	2.11	0.69
27:BW:16:ARG:NH2	27:BW:72:TYR:OH	2.25	0.69
10:BF:12:ARG:NH1	10:BF:22:GLU:O	2.26	0.69
5:AA:1327:C:OP1	16:AL:120:ASN:N	2.26	0.69
5:BA:1018:C:N4	5:BA:1150:G:O2'	2.24	0.69
6:BB:10:ASP:OD1	6:BB:11:GLN:N	2.25	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:BI:114:ARG:NH1	13:BI:186:GLU:OE2	2.26	0.69
3:A3:50:LYS:N	3:A4:188:GLU:OE2	2.26	0.69
5:BA:702:G:OP1	22:BR:16:ARG:NH2	2.24	0.69
5:AA:672:G:O6	8:AD:102:ARG:NH2	2.26	0.69
10:AF:196:LYS:NZ	10:AF:242:LEU:O	2.22	0.69
5:AA:226:G:OP1	10:AF:31:ARG:NH2	2.26	0.69
5:BA:297:G:O3'	23:BS:59:LYS:NZ	2.24	0.69
13:BI:47:THR:HG23	13:BI:49:GLY:H	1.58	0.69
8:AD:135:ARG:NH1	8:AD:135:ARG:O	2.25	0.68
5:BA:557:G:N1	5:BA:589:U:C2	2.61	0.68
5:BA:642:G:O2'	5:BA:658:A:N1	2.22	0.68
8:BD:97:ARG:O	8:BD:100:THR:OG1	2.11	0.68
11:BG:123:GLU:O	11:BG:209:ASN:ND2	2.25	0.68
11:AG:148:LYS:NZ	11:AG:150:GLY:O	2.20	0.68
19:AO:8:ASN:OD1	23:AS:62:ARG:NH1	2.27	0.68
5:BA:1220:G:OP1	5:BA:1244:C:O2'	2.11	0.68
11:BG:5:TRP:HZ2	11:BG:59:ALA:HB2	1.57	0.68
13:BI:26:VAL:HG21	13:BI:120:ILE:HB	1.76	0.68
23:AS:78:ILE:O	23:AS:108:ARG:NH2	2.25	0.68
5:BA:1216:A:OP1	7:BC:5:ARG:NH2	2.26	0.68
5:BA:1307:G:OP1	13:BI:50:ARG:NH1	2.26	0.68
5:AA:94:C:OP1	10:AF:4:LYS:N	2.27	0.68
5:BA:672:G:O2'	5:BA:673:C:OP1	2.11	0.68
5:AA:146:A:H62	5:AA:340:A:H61	1.42	0.68
5:AA:146:A:N6	5:AA:343:G:O2'	2.21	0.68
10:AF:89:ASP:OD1	10:AF:123:LYS:NZ	2.21	0.68
23:AS:45:LYS:O	23:AS:98:LYS:NZ	2.26	0.68
15:BK:43:ARG:NH1	15:BK:118:GLY:O	2.26	0.68
3:A3:187:GLU:O	3:A3:191:ALA:N	2.26	0.68
5:AA:794:A:O2'	6:AB:37:GLN:OE1	2.06	0.68
27:BW:7:GLU:OE2	27:BW:9:LYS:N	2.26	0.68
13:AI:206:GLU:OE1	13:AI:209:ARG:NH2	2.27	0.68
3:A3:214:LEU:HD23	3:A3:225:VAL:HG21	1.75	0.68
5:BA:199:A:N1	5:BA:216:G:O2'	2.27	0.68
5:BA:358:G:N1	5:BA:361:A:OP2	2.26	0.68
5:BA:1066:C:O2'	17:BM:67:ARG:NH2	2.27	0.68
11:BG:146:GLU:OE1	11:BG:146:GLU:N	2.27	0.68
20:BP:85:TYR:OH	25:BU:97:GLU:OE2	2.10	0.68
5:AA:1228:A:N3	5:AA:1286:C:O2'	2.20	0.67
3:B4:143:TYR:O	3:B4:146:THR:OG1	2.12	0.67
5:BA:926:C:OP2	5:BA:927:A:O2'	2.10	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:BF:13:LEU:O	10:BF:23:ARG:NH1	2.27	0.67
5:AA:152:G:OP1	12:AH:64:ARG:NH1	2.25	0.67
5:AA:463:G:O2'	5:AA:495:G:N3	2.28	0.67
5:BA:1301:U:O4	13:BI:78:HIS:NE2	2.27	0.67
5:AA:525:A:OP1	5:AA:773:A:N6	2.27	0.67
16:AL:31:LYS:NZ	16:AL:32:PRO:O	2.24	0.67
5:BA:934:G:O4'	5:BA:1317:G:N2	2.26	0.67
5:AA:969:A:N6	5:AA:982:U:O2	2.27	0.67
22:AR:41:ARG:NH1	22:AR:87:LEU:O	2.27	0.67
3:B3:66:ILE:O	3:B3:73:LYS:NZ	2.27	0.67
5:BA:574:A:O2'	9:BE:10:LYS:NZ	2.27	0.67
5:BA:1116:G:N7	24:BT:44:LYS:NZ	2.34	0.67
9:BE:77:LEU:HD13	9:BE:83:LEU:HD23	1.77	0.67
25:AU:24:LEU:HD21	25:AU:74:PRO:HD2	1.76	0.67
3:B3:143:TYR:O	3:B3:146:THR:OG1	2.11	0.67
5:AA:222:G:O2'	10:AF:141:ASN:ND2	2.28	0.67
5:AA:464:G:O2'	5:AA:465:C:OP2	2.11	0.67
1:A1:29:CYS:N	1:A1:35:ALA:O	2.28	0.67
3:A4:247:ASP:OD2	3:A4:250:LEU:N	2.28	0.67
5:AA:370:A:N1	5:AA:386:C:O2'	2.25	0.67
5:BA:421:U:H3	5:BA:448:A:H62	1.41	0.67
5:AA:969:A:O4'	28:AX:37:ARG:NH1	2.28	0.67
11:AG:7:GLU:OE2	11:AG:11:ARG:NH2	2.28	0.67
13:BI:212:GLU:O	13:BI:215:ARG:NH1	2.27	0.67
5:BA:693:C:HO2'	22:BR:108:HIS:HD1	1.42	0.66
5:BA:1219:C:O2'	5:BA:1243:C:O2	2.09	0.66
5:AA:1204:C:O2'	26:AV:47:GLN:NE2	2.28	0.66
12:AH:23:GLY:O	12:AH:26:THR:OG1	2.07	0.66
5:AA:446:G:O2'	5:AA:447:A:O4'	2.12	0.66
5:AA:746:A:O2'	5:AA:747:U:OP2	2.11	0.66
4:B5:19:ALA:HB2	4:B5:78:ILE:HD13	1.77	0.66
5:BA:340:A:OP2	5:BA:341:C:N4	2.20	0.66
5:BA:616:G:O2'	5:BA:790:G:OP1	2.13	0.66
5:AA:46:A:N1	5:AA:356:G:O2'	2.19	0.66
6:AB:82:LYS:NZ	6:AB:194:GLU:OE1	2.23	0.66
22:AR:96:MET:HA	22:AR:99:ILE:HD12	1.77	0.66
5:BA:1249:A:OP1	26:BV:80:ARG:NH2	2.29	0.66
20:BP:83:LYS:O	25:BU:9:ARG:NH1	2.28	0.66
5:AA:106:A:HO2'	5:AA:308:G:HO2'	1.42	0.66
5:AA:1332:C:O2'	13:AI:95:SER:O	2.07	0.66
13:BI:74:SER:OG	13:BI:163:ARG:NH1	2.28	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:BG:150:GLY:O	11:BG:153:ARG:NH1	2.29	0.66
5:AA:110:C:OP1	5:AA:558:C:O2'	2.14	0.66
2:B2:23:ILE:HD11	5:BA:849:U:C5'	2.26	0.66
5:AA:557:G:N1	5:AA:589:U:C2	2.64	0.66
5:AA:1307:G:O2'	5:AA:1333:G:N1	2.27	0.66
7:BC:196:ILE:O	24:BT:20:TYR:OH	2.13	0.65
13:BI:9:PHE:CE1	16:BL:46:LEU:HD22	2.31	0.65
11:AG:16:TRP:O	11:AG:27:LYS:NZ	2.27	0.65
5:AA:234:G:OP1	23:AS:66:ARG:NH1	2.29	0.65
5:AA:104:A:OP1	15:AK:11:LYS:NZ	2.22	0.65
5:AA:607:U:C5	14:AJ:58:ALA:HB2	2.32	0.65
5:AA:1275:U:N3	5:AA:1279:A:N6	2.45	0.65
19:AO:38:LYS:O	19:AO:42:ASP:N	2.30	0.65
4:A5:37:ASN:OD1	4:A5:38:GLU:N	2.29	0.65
13:BI:38:ASN:ND2	13:BI:60:ASN:O	2.29	0.65
5:AA:895:C:O2'	5:AA:1342:C:N4	2.28	0.65
5:AA:1049:U:O2'	5:AA:1129:A:N3	2.29	0.65
5:AA:398:C:OP1	9:AE:43:LYS:NZ	2.24	0.65
2:A2:6:ARG:NH2	5:AA:844:G:O3'	2.30	0.65
5:AA:542:G:O3'	14:AJ:31:SER:OG	2.14	0.65
5:AA:1007:A:N6	5:AA:1160:C:O2	2.30	0.65
21:AQ:31:ILE:HG23	21:AQ:36:LEU:HD13	1.77	0.65
13:BI:17:VAL:HG21	13:BI:120:ILE:HD11	1.79	0.65
1:B1:23:HIS:O	1:B1:44:ARG:NH1	2.30	0.64
5:BA:564:C:OP1	9:BE:5:LYS:NZ	2.23	0.64
9:BE:59:LEU:O	9:BE:62:ARG:NH2	2.30	0.64
3:A3:84:LEU:HD21	3:A3:204:VAL:HG11	1.79	0.64
23:AS:87:LEU:HD13	23:AS:104:ALA:HB3	1.78	0.64
5:BA:975:A:O2'	5:BA:976:A:OP1	2.14	0.64
15:BK:31:GLU:O	15:BK:56:ARG:NH1	2.30	0.64
3:A3:233:ARG:NH1	3:A3:263:THR:O	2.30	0.64
5:AA:371:U:O2'	10:AF:28:TRP:O	2.15	0.64
10:AF:185:VAL:CG2	10:AF:199:ILE:HD11	2.27	0.64
5:AA:559:G:N2	5:AA:587:G:OP2	2.31	0.64
2:B2:31:LYS:O	2:B2:35:GLY:N	2.30	0.64
5:BA:148:C:O3'	12:BH:105:LYS:NZ	2.30	0.64
5:BA:896:A:N3	5:BA:1338:C:N4	2.46	0.64
5:BA:1090:C:O2'	26:BV:130:ASP:OD2	2.15	0.64
5:BA:1306:A:O2'	13:BI:50:ARG:NE	2.30	0.64
5:AA:31:U:C2	5:AA:501:G:N1	2.66	0.64
5:AA:111:G:O2'	5:AA:112:G:OP1	2.13	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AA:1004:U:O2	5:AA:1166:G:O6	2.15	0.64
18:AN:25:ASN:OD1	18:AN:26:THR:N	2.30	0.64
5:BA:934:G:OP2	5:BA:1323:A:N6	2.31	0.64
22:BR:104:ASN:OD1	22:BR:105:LEU:N	2.31	0.64
1:B1:21:ARG:NH1	11:BG:121:ILE:O	2.31	0.64
5:BA:934:G:H21	21:BQ:31:ILE:HD12	1.61	0.64
17:BM:17:ASP:OD1	17:BM:71:ARG:NH2	2.30	0.64
5:BA:883:G:N2	5:BA:1458:A:OP1	2.30	0.64
5:AA:1153:G:O3'	11:AG:80:ARG:NH2	2.31	0.63
9:AE:67:GLU:OE1	9:AE:70:ARG:NH1	2.31	0.63
26:AV:72:ARG:O	26:AV:75:THR:OG1	2.15	0.63
3:B3:160:ILE:HD11	3:B3:176:LEU:HB3	1.78	0.63
5:AA:1275:U:OP2	25:AU:38:ARG:NH2	2.31	0.63
5:AA:1307:G:N2	5:AA:1334:A:OP2	2.30	0.63
5:BA:344:G:OP1	12:BH:106:THR:OG1	2.17	0.63
5:AA:1167:C:OP1	7:AC:172:LYS:NZ	2.32	0.63
5:AA:1266:A:N7	5:AA:1291:G:O2'	2.31	0.63
6:BB:131:VAL:HG21	6:BB:149:TYR:CD1	2.34	0.63
8:BD:45:ASN:N	8:BD:70:VAL:O	2.32	0.63
3:A4:232:LEU:HD22	3:A4:260:LEU:HD21	1.80	0.63
5:AA:471:G:N2	19:AO:65:PRO:O	2.31	0.63
5:AA:1171:G:O2'	5:AA:1173:A:N6	2.32	0.63
5:BA:1276:G:O6	25:BU:38:ARG:NH1	2.32	0.63
3:A4:186:ILE:HD11	3:A4:200:GLY:HA3	1.80	0.63
5:AA:885:G:O2'	5:AA:1487:U:O4'	2.16	0.63
11:AG:124:ILE:HD13	11:AG:178:ALA:HB1	1.79	0.63
17:AM:86:MET:SD	17:AM:87:ARG:NH1	2.72	0.63
9:BE:36:LYS:N	9:BE:40:GLU:OE2	2.32	0.63
1:A1:41:GLU:OE1	6:AB:149:TYR:OH	2.15	0.63
5:AA:262:G:O2'	5:AA:263:C:O5'	2.17	0.63
5:BA:112:G:H21	5:BA:229:G:H1	1.46	0.63
5:AA:924:U:O2'	5:AA:925:U:OP2	2.13	0.63
5:BA:778:G:N2	14:BJ:9:ASN:OD1	2.31	0.63
3:A3:35:VAL:HG23	3:A3:82:ILE:HD11	1.79	0.63
3:A4:213:TYR:CZ	3:A4:214:LEU:HD13	2.33	0.63
5:BA:176:U:O4	5:BA:187:C:N3	2.32	0.63
5:BA:730:G:N2	5:BA:756:A:OP2	2.29	0.63
6:BB:169:TRP:NE1	6:BB:190:ILE:O	2.30	0.63
23:BS:16:CYS:SG	23:BS:24:HIS:ND1	2.66	0.63
3:A4:268:THR:OG1	3:A4:270:PHE:O	2.13	0.63
5:AA:320:G:N1	5:AA:323:A:OP2	2.31	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AA:964:A:N6	5:AA:989:C:HO2'	1.95	0.63
5:BA:1195:U:O2'	26:BV:84:GLY:O	2.14	0.63
5:AA:672:G:O2'	5:AA:673:C:OP1	2.16	0.62
14:AJ:50:PHE:HB3	14:AJ:63:VAL:HG22	1.80	0.62
15:AK:67:ASP:OD2	15:AK:69:SER:OG	2.10	0.62
5:AA:640:U:O2'	5:AA:641:A:O5'	2.14	0.62
6:AB:198:LYS:NZ	6:AB:199:ILE:O	2.30	0.62
3:B3:268:THR:O	3:B3:270:PHE:N	2.31	0.62
5:BA:1076:G:O2'	5:BA:1077:U:O5'	2.16	0.62
5:BA:1117:A:OP2	24:BT:32:LYS:NZ	2.32	0.62
5:AA:520:G:OP2	19:AO:5:LYS:NZ	2.29	0.62
5:AA:1250:C:OP1	13:AI:99:LYS:NZ	2.23	0.62
11:AG:166:VAL:O	11:AG:185:SER:OG	2.11	0.62
19:AO:103:VAL:HG23	19:AO:105:ILE:HD11	1.80	0.62
3:B4:11:SER:OG	3:B4:27:ARG:NH1	2.32	0.62
4:A5:57:VAL:HG12	4:A5:59:PRO:HD2	1.80	0.62
5:BA:1298:G:OP2	13:BI:80:LYS:NZ	2.28	0.62
15:AK:86:ASN:OD1	15:AK:87:ARG:N	2.33	0.62
5:BA:104:A:OP1	15:BK:11:LYS:NZ	2.31	0.62
9:BE:85:GLU:OE2	9:BE:146:LYS:NZ	2.32	0.62
17:BM:33:ARG:NH2	17:BM:34:MET:O	2.32	0.62
9:AE:130:ILE:HD12	9:AE:153:THR:O	1.99	0.62
10:AF:134:LYS:O	10:AF:137:ARG:NH1	2.32	0.62
18:BN:107:ARG:NH2	30:BZ:60:THR:OG1	2.33	0.62
5:AA:1248:A:N6	5:AA:1331:G:O2'	2.22	0.62
5:BA:1228:A:OP1	26:BV:99:ARG:NH2	2.33	0.62
12:BH:34:ILE:HD11	12:BH:74:MET:HG2	1.82	0.62
5:AA:939:C:O2	21:AQ:17:GLY:N	2.33	0.61
20:AP:68:ASP:O	20:AP:72:HIS:ND1	2.32	0.61
4:B5:92:ILE:HD11	4:B5:96:ALA:HB2	1.82	0.61
27:BW:22:GLU:HB3	27:BW:64:ILE:HD11	1.82	0.61
5:AA:1081:C:N4	5:AA:1099:A:N7	2.47	0.61
11:AG:67:ASP:OD2	11:AG:194:THR:OG1	2.08	0.61
11:AG:86:LEU:HD11	11:AG:98:LEU:HD11	1.82	0.61
19:BO:51:ARG:HD2	19:BO:78:ILE:HD12	1.82	0.61
5:AA:898:G:O2'	13:AI:163:ARG:NH2	2.34	0.61
5:AA:1340:U:O2'	5:AA:1341:C:OP2	2.12	0.61
5:BA:370:A:N1	5:BA:386:C:O2'	2.26	0.61
9:BE:61:ALA:O	9:BE:62:ARG:NE	2.33	0.61
18:BN:101:ALA:O	18:BN:105:LEU:HD22	2.00	0.61
23:BS:60:TYR:O	23:BS:62:ARG:NE	2.33	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A3:32:GLU:OE1	3:A3:32:GLU:N	2.32	0.61
5:AA:1053:A:N7	6:AB:125:GLN:NE2	2.48	0.61
18:AN:42:TRP:NE1	18:AN:70:GLU:OE1	2.33	0.61
5:BA:429:A:O3'	27:BW:32:SER:OG	2.18	0.61
5:BA:516:A:OP2	19:BO:20:ARG:NH2	2.34	0.61
5:BA:1193:G:OP1	16:BL:121:ARG:NH2	2.34	0.61
3:A4:294:GLN:O	3:A4:298:GLY:N	2.33	0.61
5:AA:939:C:O2'	5:AA:940:U:OP1	2.11	0.61
1:A1:28:ILE:HD11	1:A1:33:GLY:C	2.21	0.61
3:A4:143:TYR:O	3:A4:146:THR:OG1	2.15	0.61
2:A2:21:LYS:NZ	5:AA:1468:A:N7	2.48	0.61
5:AA:533:C:OP1	22:AR:5:HIS:ND1	2.32	0.61
5:AA:693:C:O2'	22:AR:108:HIS:ND1	2.23	0.61
3:B4:134:LEU:O	3:B4:140:ARG:NH1	2.33	0.61
5:BA:557:G:C2	5:BA:589:U:O2	2.53	0.61
5:AA:1063:A:OP2	5:AA:1064:C:N4	2.33	0.61
22:AR:82:LEU:O	22:AR:88:ALA:N	2.34	0.61
1:A1:28:ILE:HD12	1:A1:29:CYS:H	1.66	0.61
3:A4:113:GLU:OE1	3:A4:128:TYR:OH	2.12	0.61
5:AA:776:C:O2'	22:AR:7:ARG:NH2	2.34	0.61
5:BA:970:G:N1	5:BA:981:U:O4	2.33	0.61
8:AD:124:ILE:O	8:AD:181:ARG:N	2.34	0.61
11:AG:13:LEU:O	11:AG:27:LYS:NZ	2.26	0.61
5:BA:1318:U:OP2	5:BA:1319:C:N4	2.34	0.61
22:BR:87:LEU:HD12	22:BR:87:LEU:O	1.99	0.61
27:BW:78:MET:N	27:BW:78:MET:SD	2.73	0.61
3:A4:262:ASN:O	3:A4:262:ASN:ND2	2.34	0.60
5:AA:1471:G:N2	5:AA:1474:A:OP2	2.30	0.60
13:BI:45:PRO:HB3	13:BI:64:VAL:HG23	1.83	0.60
5:AA:365:C:OP2	5:AA:384:G:N1	2.31	0.60
5:AA:641:A:O2'	5:AA:642:G:OP2	2.13	0.60
14:AJ:23:ARG:O	14:AJ:65:LEU:HD12	2.01	0.60
3:B4:273:GLU:OE1	3:B4:273:GLU:N	2.34	0.60
5:BA:1120:G:OP1	24:BT:5:ARG:NH2	2.32	0.60
17:BM:1:MET:SD	17:BM:1:MET:N	2.72	0.60
10:AF:105:ASN:N	10:AF:109:LYS:O	2.34	0.60
22:AR:93:GLU:N	22:AR:93:GLU:OE2	2.33	0.60
5:BA:762:G:OP2	22:BR:114:LYS:NZ	2.26	0.60
5:AA:125:G:H5'	10:AF:149:ILE:HG21	1.82	0.60
11:AG:3:GLN:N	11:AG:3:GLN:OE1	2.34	0.60
5:AA:1262:U:O2'	5:AA:1263:C:OP1	2.14	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AA:1333:G:OP1	13:AI:46:HIS:NE2	2.34	0.60
10:AF:62:ALA:O	10:AF:66:LEU:HD22	2.02	0.60
5:BA:110:C:OP1	5:BA:558:C:O2'	2.19	0.60
7:BC:84:GLU:O	7:BC:86:LYS:NZ	2.26	0.60
26:BV:30:GLU:OE1	26:BV:30:GLU:N	2.34	0.60
3:A3:174:ILE:O	3:A3:177:SER:OG	2.15	0.60
3:A3:65:LYS:O	3:A3:67:LYS:NZ	2.33	0.60
10:AF:195:ARG:NH2	10:AF:221:GLU:OE1	2.35	0.60
13:AI:29:ARG:N	13:AI:128:GLU:OE2	2.35	0.60
25:AU:68:ARG:NH2	25:AU:104:GLY:O	2.35	0.60
5:BA:151:G:O2'	12:BH:64:ARG:NH1	2.34	0.60
12:BH:32:LYS:HB2	12:BH:112:ILE:HD12	1.84	0.60
1:B1:13:SER:OG	1:B1:43:CYS:SG	2.60	0.60
5:BA:93:A:O2'	10:BF:4:LYS:O	2.08	0.60
5:BA:1269:G:N1	5:BA:1289:G:O6	2.35	0.60
10:BF:183:ALA:O	10:BF:199:ILE:HD12	2.02	0.60
5:AA:1197:C:HO2'	5:AA:1260:G:H22	1.44	0.59
9:AE:38:LYS:HA	9:AE:41:LEU:HD12	1.84	0.59
23:AS:84:ASP:OD1	23:AS:109:ALA:N	2.35	0.59
1:B1:50:TYR:OH	6:BB:151:ASP:O	2.20	0.59
5:BA:16:G:H21	5:BA:872:A:N6	1.90	0.59
13:BI:24:GLU:OE1	13:BI:24:GLU:N	2.35	0.59
14:BJ:37:VAL:HG23	14:BJ:103:ILE:HG21	1.84	0.59
14:AJ:25:VAL:HG13	14:AJ:65:LEU:HD11	1.83	0.59
22:AR:126:GLU:OE1	22:AR:130:ARG:NH2	2.35	0.59
12:BH:88:LEU:HD22	12:BH:94:PHE:HB3	1.84	0.59
5:AA:706:G:HO2'	5:AA:707:A:P	2.24	0.59
11:AG:96:VAL:HG12	11:AG:124:ILE:HD11	1.84	0.59
5:BA:274:G:OP2	23:BS:69:LYS:NZ	2.34	0.59
5:BA:342:G:O2'	12:BH:83:ARG:NH1	2.35	0.59
5:AA:181:G:O6	10:AF:208:GLY:N	2.35	0.59
5:AA:743:U:O2'	5:AA:745:G:N7	2.31	0.59
5:AA:1265:G:N1	5:AA:1292:A:OP2	2.35	0.59
5:BA:777:G:O2'	14:BJ:2:THR:N	2.28	0.59
5:BA:899:G:OP1	13:BI:163:ARG:NH2	2.35	0.59
5:BA:1341:C:HO2'	5:BA:1342:C:H6	1.49	0.59
5:AA:341:C:O2	5:AA:342:G:N1	2.36	0.59
5:AA:983:G:HO2'	5:AA:984:C:C1'	2.13	0.59
5:AA:1238:G:OP2	5:AA:1238:G:N2	2.25	0.59
12:AH:67:THR:OG1	12:AH:118:GLN:OE1	2.16	0.59
12:BH:63:ILE:HA	12:BH:121:VAL:HG12	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AA:1160:C:O2'	5:AA:1165:U:O4	2.18	0.59
30:AZ:42:ARG:NE	30:AZ:64:ALA:O	2.36	0.59
5:BA:1007:A:N6	5:BA:1160:C:C2	2.71	0.59
5:BA:1333:G:OP1	13:BI:46:HIS:NE2	2.33	0.59
27:BW:85:TYR:HA	27:BW:88:ILE:HD12	1.85	0.59
5:AA:408:C:O2'	5:AA:409:C:OP1	2.18	0.59
5:AA:695:G:H5'	22:AR:105:LEU:HD13	1.85	0.59
6:BB:87:THR:OG1	6:BB:179:ARG:NH1	2.35	0.59
20:BP:37:THR:HG21	26:BV:44:LEU:HD23	1.85	0.59
5:AA:671:C:HO2'	5:AA:688:C:H6	1.50	0.59
20:AP:113:ARG:CD	20:AP:118:ILE:HD11	2.33	0.59
22:AR:63:VAL:HG21	22:AR:78:ILE:HD11	1.84	0.59
3:B3:98:GLU:OE2	3:B3:98:GLU:N	2.35	0.59
5:BA:311:A:OP2	15:BK:22:LYS:NZ	2.36	0.59
5:BA:1019:A:O2'	5:BA:1045:A:O3'	2.21	0.59
5:BA:1209:C:O2	5:BA:1248:A:N6	2.34	0.59
5:BA:1209:C:OP1	16:BL:74:GLN:NE2	2.36	0.59
11:AG:68:ILE:HG23	11:AG:85:VAL:HG22	1.83	0.59
6:BB:60:ALA:HB1	6:BB:179:ARG:HG3	1.85	0.59
15:BK:3:ILE:O	15:BK:29:GLY:N	2.34	0.59
5:AA:43:A:H5"	5:AA:361:A:H62	1.68	0.59
5:AA:628:G:N2	18:AN:124:ASP:OD2	2.36	0.59
5:AA:977:G:O2'	5:AA:978:G:OP2	2.16	0.59
5:AA:1196:A:O2'	5:AA:1294:G:N2	2.34	0.59
5:BA:750:C:O2'	18:BN:135:ARG:NH2	2.36	0.59
5:BA:1226:G:N7	26:BV:99:ARG:NH1	2.51	0.59
5:AA:291:G:OP1	9:AE:8:ARG:NH1	2.36	0.58
5:AA:305:C:OP1	10:AF:11:LYS:NZ	2.26	0.58
20:AP:21:LEU:HD13	20:AP:54:LEU:HD11	1.84	0.58
29:AY:10:ARG:O	29:AY:12:ARG:NH2	2.34	0.58
2:A2:3:ARG:NH1	5:AA:768:A:OP1	2.36	0.58
3:A3:144:ARG:NE	3:A3:247:ASP:OD1	2.34	0.58
5:AA:272:C:OP1	23:AS:40:SER:OG	2.20	0.58
5:AA:1220:G:O2'	5:AA:1235:A:N6	2.37	0.58
20:AP:81:ARG:NE	20:AP:84:ASP:OD1	2.35	0.58
3:B4:39:ILE:O	3:B4:105:LYS:NZ	2.31	0.58
5:BA:561:A:O2'	10:BF:23:ARG:NH1	2.36	0.58
5:AA:115:A:O2'	5:AA:116:C:O5'	2.21	0.58
5:BA:617:A:OP1	8:BD:132:SER:OG	2.12	0.58
5:BA:1188:C:N4	20:BP:132:ARG:O	2.36	0.58
5:BA:1272:G:OP2	25:BU:30:ALA:N	2.37	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:BD:51:THR:OG1	8:BD:54:ASP:OD2	2.18	0.58
3:A3:144:ARG:NH1	3:A3:239:ASP:OD2	2.37	0.58
16:AL:46:LEU:CD2	16:AL:50:ILE:HD11	2.33	0.58
26:BV:15:ARG:NH1	26:BV:18:GLN:OE1	2.36	0.58
5:AA:293:G:N2	5:AA:296:A:OP2	2.32	0.58
8:AD:119:VAL:HG22	8:AD:188:ILE:HG12	1.85	0.58
10:AF:65:ILE:HG22	10:AF:71:PHE:HE1	1.69	0.58
19:AO:57:LYS:NZ	19:AO:97:ILE:O	2.28	0.58
5:BA:799:C:OP1	8:BD:175:LYS:NZ	2.36	0.58
5:BA:942:A:O2'	5:BA:1002:G:OP2	2.18	0.58
5:AA:435:A:OP2	27:AW:89:ARG:NH2	2.36	0.58
8:AD:117:LEU:HD11	8:AD:188:ILE:HG23	1.86	0.58
10:AF:185:VAL:HG21	10:AF:199:ILE:HD11	1.84	0.58
23:AS:46:THR:HG23	23:AS:98:LYS:HE2	1.86	0.58
25:BU:55:LYS:NZ	25:BU:75:GLU:O	2.27	0.58
6:AB:59:LEU:HD12	6:AB:67:ILE:HD13	1.86	0.58
22:AR:94:ASP:OD1	22:AR:94:ASP:N	2.35	0.58
24:AT:5:ARG:HD2	24:AT:9:ILE:HD11	1.85	0.58
5:BA:111:G:O2'	5:BA:112:G:OP1	2.19	0.58
10:BF:127:ILE:HD12	10:BF:162:TYR:HB2	1.86	0.58
14:BJ:38:LEU:HD13	14:BJ:61:TYR:CE2	2.37	0.58
20:BP:10:VAL:HG12	20:BP:59:VAL:HG13	1.85	0.58
5:AA:557:G:C2	5:AA:589:U:O2	2.56	0.58
5:AA:1483:U:O2'	5:AA:1484:C:OP2	2.19	0.58
3:B4:157:LYS:HB3	3:B4:183:ILE:HG21	1.85	0.58
3:A4:195:LYS:NZ	5:BA:655:A:N3	2.52	0.58
27:BW:8:ILE:HG12	27:BW:19:ILE:HG22	1.86	0.58
3:A3:219:GLU:OE1	3:A3:219:GLU:N	2.37	0.58
5:AA:1413:G:OP1	12:AH:89:SER:OG	2.17	0.58
3:B4:4:VAL:HG21	3:B4:201:LEU:HD11	1.85	0.58
4:B5:69:LEU:HD13	28:BX:15:VAL:HG11	1.86	0.58
5:BA:56:A:N1	5:BA:91:G:O2'	2.30	0.58
5:BA:1281:U:O2'	25:BU:110:ARG:NH2	2.37	0.58
5:BA:1413:G:OP1	12:BH:89:SER:OG	2.22	0.58
3:A3:23:LYS:NZ	5:AA:244:G:N7	2.52	0.57
3:A4:214:LEU:HD12	3:A4:227:PRO:HA	1.86	0.57
25:AU:68:ARG:O	25:AU:104:GLY:N	2.36	0.57
5:BA:1215:G:N2	5:BA:1219:C:O2	2.30	0.57
2:A2:6:ARG:NE	5:AA:845:G:OP1	2.36	0.57
30:AZ:45:VAL:HG11	30:AZ:49:VAL:HB	1.85	0.57
22:AR:48:ALA:O	22:AR:52:THR:HG23	2.03	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AS:3:ARG:NH1	23:AS:25:GLY:O	2.37	0.57
19:BO:98:ASP:OD2	19:BO:144:LYS:NZ	2.31	0.57
29:BY:3:LYS:NZ	29:BY:4:PRO:O	2.35	0.57
3:A3:271:SER:OG	3:A3:273:GLU:OE1	2.17	0.57
5:AA:1275:U:O4	25:AU:31:ARG:NH2	2.33	0.57
13:AI:9:PHE:CE1	16:AL:46:LEU:HD13	2.40	0.57
23:AS:21:CYS:SG	23:AS:24:HIS:N	2.76	0.57
5:BA:483:G:N2	5:BA:483:G:OP2	2.37	0.57
5:BA:952:A:N6	5:BA:996:A:O2'	2.38	0.57
5:BA:1197:C:O2'	5:BA:1260:G:N2	2.30	0.57
23:AS:20:LYS:HE3	23:AS:27:LEU:HD13	1.85	0.57
5:BA:1340:U:O2'	5:BA:1341:C:OP2	2.17	0.57
24:BT:25:THR:O	24:BT:31:ASN:ND2	2.37	0.57
3:A4:20:LYS:NZ	3:A4:210:SER:O	2.23	0.57
5:AA:369:A:N6	5:AA:387:G:N3	2.51	0.57
5:BA:352:A:O2'	5:BA:364:U:O3'	2.18	0.57
7:BC:91:ASN:OD1	7:BC:93:LYS:N	2.36	0.57
2:A2:6:ARG:NH2	5:AA:873:A:O2'	2.38	0.57
3:A4:172:LEU:O	3:A4:176:LEU:HD12	2.05	0.57
5:AA:795:G:O4'	6:AB:37:GLN:NE2	2.38	0.57
6:AB:50:GLU:O	6:AB:54:VAL:HG23	2.05	0.57
11:AG:131:TRP:O	11:AG:134:ARG:NH2	2.35	0.57
3:B3:50:LYS:O	3:B3:54:ILE:HD12	2.04	0.57
2:A2:10:LYS:NZ	5:AA:1464:C:OP1	2.35	0.57
5:AA:93:A:O2'	10:AF:4:LYS:O	2.08	0.57
5:BA:91:G:H3'	5:BA:92:G:H21	1.70	0.57
3:A3:215:ASP:N	3:A3:215:ASP:OD1	2.34	0.57
5:AA:371:U:OP1	10:AF:50:ARG:NH2	2.38	0.57
5:AA:615:G:O6	5:AA:698:A:C6	2.58	0.57
5:AA:1296:U:N3	13:AI:89:GLU:OE2	2.38	0.57
6:AB:97:LEU:O	6:AB:100:THR:OG1	2.23	0.57
8:BD:126:MET:N	8:BD:126:MET:SD	2.77	0.57
9:BE:83:LEU:HD11	9:BE:95:LEU:HD21	1.87	0.57
20:BP:83:LYS:N	20:BP:90:ASP:OD1	2.38	0.57
5:AA:101:G:N2	15:AK:20:ALA:HB1	2.20	0.57
8:AD:120:MET:N	8:AD:120:MET:SD	2.78	0.57
12:AH:48:ASN:OD1	12:AH:55:PHE:N	2.38	0.57
5:BA:11:A:N3	5:BA:1032:A:O2'	2.28	0.57
5:BA:123:U:OP1	10:BF:76:ARG:NH1	2.38	0.57
5:BA:1296:U:N3	13:BI:89:GLU:OE2	2.37	0.57
8:BD:49:GLU:OE2	8:BD:65:LYS:NZ	2.37	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:46:LEU:HD13	1:A1:48:LYS:NZ	2.20	0.56
5:BA:1436:U:HO2'	5:BA:1437:G:P	2.28	0.56
6:BB:161:ARG:NH1	6:BB:197:MET:O	2.38	0.56
14:BJ:23:ARG:O	14:BJ:65:LEU:HD12	2.05	0.56
30:BZ:42:ARG:NE	30:BZ:64:ALA:O	2.38	0.56
5:AA:1062:G:N2	7:AC:191:ASP:OD2	2.37	0.56
15:AK:65:VAL:HG11	15:AK:105:ILE:HD12	1.86	0.56
5:BA:291:G:OP1	9:BE:8:ARG:NH1	2.38	0.56
5:AA:985:C:O2'	5:AA:986:G:OP1	2.20	0.56
5:AA:1281:U:O2'	25:AU:110:ARG:NH2	2.38	0.56
2:B2:23:ILE:HD11	5:BA:849:U:H5"	1.86	0.56
3:B3:230:ARG:NH1	3:B3:265:ARG:O	2.38	0.56
5:BA:106:A:OP2	15:BK:7:ARG:NH2	2.38	0.56
5:BA:584:C:O2'	5:BA:585:U:OP1	2.15	0.56
5:BA:820:G:OP1	11:BG:148:LYS:NZ	2.34	0.56
8:BD:25:ASP:OD1	8:BD:26:PHE:N	2.38	0.56
1:A1:31:ASN:O	6:AB:57:LYS:NZ	2.38	0.56
5:AA:1055:C:OP1	6:AB:95:ARG:NH1	2.39	0.56
5:AA:1273:G:OP2	25:AU:33:ARG:NH2	2.39	0.56
5:AA:1392:G:HO2'	5:AA:1423:A:H61	1.49	0.56
11:AG:126:ARG:NH2	11:AG:226:GLY:O	2.33	0.56
5:BA:1260:G:O2'	5:BA:1261:U:OP2	2.18	0.56
13:BI:40:GLU:N	13:BI:40:GLU:OE1	2.38	0.56
23:BS:111:GLU:OE1	23:BS:111:GLU:N	2.38	0.56
5:AA:1036:G:OP2	5:AA:1037:U:O2'	2.18	0.56
13:AI:81:VAL:O	13:AI:84:HIS:ND1	2.38	0.56
1:B1:8:ILE:HD13	11:BG:39:ARG:HH21	1.70	0.56
5:BA:227:C:OP2	10:BF:7:LYS:NZ	2.38	0.56
10:BF:117:GLU:OE1	10:BF:117:GLU:N	2.37	0.56
5:AA:1207:G:OP1	26:AV:61:ARG:NH1	2.38	0.56
5:BA:1210:A:H61	5:BA:1314:C:H1'	1.70	0.56
21:BQ:52:PHE:O	21:BQ:53:ARG:NE	2.39	0.56
5:AA:606:U:O4	5:AA:706:G:O2'	2.24	0.56
5:AA:681:G:N2	5:AA:684:G:OP2	2.35	0.56
5:AA:718:G:O3'	22:AR:116:LEU:HD13	2.05	0.56
5:BA:967:C:O2	5:BA:983:G:N2	2.39	0.56
11:BG:126:ARG:NH2	11:BG:226:GLY:O	2.36	0.56
17:BM:5:ARG:HD2	17:BM:101:ILE:HD11	1.88	0.56
5:BA:474:G:OP2	19:BO:71:LYS:NZ	2.31	0.56
5:BA:746:A:O2'	5:BA:747:U:OP2	2.16	0.56
14:BJ:23:ARG:NH1	14:BJ:65:LEU:O	2.39	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AA:1326:G:OP1	16:AL:121:ARG:NH2	2.37	0.56
3:B3:35:VAL:HB	3:B3:82:ILE:HD11	1.86	0.56
5:BA:1266:A:N6	5:BA:1291:G:O2'	2.38	0.56
5:AA:991:C:N4	5:AA:992:G:O6	2.39	0.56
3:B4:16:LEU:O	3:B4:16:LEU:HD23	2.06	0.56
5:BA:276:A:O2'	5:BA:277:G:OP1	2.21	0.56
5:BA:1060:G:OP1	7:BC:154:VAL:N	2.39	0.56
3:A4:3:VAL:O	3:A4:5:GLY:N	2.39	0.55
3:B4:219:GLU:OE1	3:B4:219:GLU:N	2.39	0.55
8:BD:58:ASP:OD2	8:BD:60:THR:OG1	2.22	0.55
5:AA:135:U:O2'	5:AA:136:A:O5'	2.20	0.55
10:BF:105:ASN:OD1	10:BF:106:ARG:N	2.38	0.55
1:A1:32:CYS:SG	1:A1:33:GLY:N	2.80	0.55
13:AI:55:HIS:O	13:AI:58:LYS:NZ	2.20	0.55
3:B3:78:ARG:O	3:B3:81:SER:OG	2.20	0.55
3:B3:268:THR:OG1	3:B3:272:GLU:OE2	2.25	0.55
4:B5:84:LYS:NZ	4:B5:93:GLU:O	2.38	0.55
5:BA:772:G:N2	5:BA:774:U:O2'	2.40	0.55
5:BA:1378:A:N6	5:BA:1437:G:O2'	2.40	0.55
18:BN:118:VAL:O	18:BN:118:VAL:HG12	2.06	0.55
20:BP:68:ASP:O	20:BP:72:HIS:ND1	2.39	0.55
3:A3:140:ARG:NH2	3:A3:239:ASP:OD1	2.40	0.55
4:B5:114:ILE:O	4:B5:118:VAL:N	2.38	0.55
3:A4:152:ASP:OD2	3:A4:222:LYS:NZ	2.28	0.55
5:AA:640:U:HO2'	5:AA:641:A:P	2.30	0.55
13:AI:176:ASN:OD1	13:AI:177:LYS:N	2.39	0.55
5:BA:515:U:O2'	19:BO:20:ARG:NH2	2.40	0.55
5:BA:1180:G:O2'	25:BU:84:HIS:O	2.24	0.55
5:AA:893:U:N3	5:AA:1015:C:OP1	2.39	0.55
5:BA:933:G:OP2	21:BQ:40:ARG:NH1	2.39	0.55
5:AA:27:C:O2	19:AO:49:GLN:NE2	2.39	0.55
5:AA:793:G:OP1	29:AY:51:LYS:NZ	2.37	0.55
10:AF:137:ARG:HB3	10:AF:149:ILE:HD11	1.89	0.55
11:AG:218:ILE:HG23	11:AG:223:ILE:HB	1.88	0.55
5:BA:803:C:O3'	8:BD:127:ARG:NH2	2.39	0.55
10:AF:65:ILE:HG22	10:AF:71:PHE:CE1	2.42	0.55
5:BA:681:G:N2	5:BA:684:G:OP2	2.37	0.55
5:BA:963:A:H62	5:BA:988:A:H1'	1.70	0.55
5:BA:1296:U:O2'	13:BI:85:PHE:O	2.23	0.55
12:BH:70:ASP:OD2	12:BH:83:ARG:NH2	2.40	0.55
30:BZ:59:GLU:OE1	30:BZ:62:ARG:NE	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AD:93:ARG:NH1	8:AD:93:ARG:O	2.40	0.55
3:B3:94:VAL:HG12	3:B3:103:VAL:HG12	1.89	0.55
5:BA:261:G:N1	15:BK:5:GLN:OE1	2.40	0.55
5:BA:1220:G:H21	5:BA:1235:A:H62	1.53	0.55
3:A3:64:ASN:ND2	5:AA:764:C:OP1	2.39	0.55
5:AA:575:A:O2'	9:AE:7:GLN:OE1	2.25	0.55
5:AA:1188:C:N4	20:AP:132:ARG:O	2.40	0.55
14:AJ:28:LYS:HZ3	14:AJ:58:ALA:HB3	1.71	0.55
22:AR:135:TYR:OH	22:AR:139:LYS:NZ	2.21	0.55
5:BA:1338:C:N4	30:BZ:23:ASP:OD1	2.39	0.55
1:A1:29:CYS:HB2	1:A1:35:ALA:HB3	1.88	0.54
3:A4:150:VAL:HG23	3:A4:155:GLY:HA3	1.89	0.54
12:AH:65:GLY:O	12:AH:120:ASN:N	2.38	0.54
5:BA:718:G:H4'	22:BR:116:LEU:HD22	1.89	0.54
5:BA:1183:C:OP2	25:BU:110:ARG:NH2	2.40	0.54
18:BN:47:VAL:HG23	18:BN:48:VAL:HG13	1.89	0.54
27:AW:33:ARG:NH1	27:AW:90:ASP:OD1	2.40	0.54
5:BA:908:G:HO2'	5:BA:930:G:H1	1.55	0.54
11:BG:165:LEU:HD12	11:BG:183:VAL:HG12	1.89	0.54
5:AA:1262:U:HO2'	5:AA:1263:C:P	2.29	0.54
5:AA:1264:G:N2	5:AA:1294:G:O6	2.40	0.54
6:AB:100:THR:N	6:AB:129:GLU:OE1	2.40	0.54
10:AF:180:GLU:OE1	10:AF:180:GLU:N	2.40	0.54
5:BA:786:G:O2'	5:BA:787:U:O4'	2.20	0.54
2:A2:26:LEU:HD12	2:A2:29:GLN:HE21	1.72	0.54
5:AA:718:G:H4'	22:AR:116:LEU:HD22	1.88	0.54
5:AA:1313:G:OP1	26:AV:80:ARG:NH1	2.38	0.54
5:BA:324:C:OP1	10:BF:4:LYS:NZ	2.37	0.54
5:BA:1279:A:O2'	5:BA:1282:C:O2'	2.24	0.54
6:BB:172:ALA:HA	6:BB:175:ILE:HD12	1.90	0.54
5:AA:258:A:OP1	15:AK:30:ARG:NH2	2.38	0.54
5:AA:1274:C:OP2	25:AU:34:ARG:NE	2.38	0.54
2:B2:3:ARG:NH1	5:BA:768:A:OP1	2.37	0.54
5:BA:242:A:N6	5:BA:277:G:O2'	2.41	0.54
11:BG:20:THR:HG22	11:BG:46:GLU:OE2	2.07	0.54
5:AA:1017:U:N3	5:AA:1150:G:O4'	2.40	0.54
3:B3:201:LEU:HA	3:B3:204:VAL:HG12	1.89	0.54
10:BF:185:VAL:HG23	10:BF:199:ILE:HD11	1.90	0.54
11:BG:16:TRP:O	11:BG:27:LYS:NZ	2.39	0.54
16:BL:46:LEU:HD23	16:BL:50:ILE:HD11	1.89	0.54
17:BM:8:ILE:HG22	17:BM:96:ILE:HG12	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A3:84:LEU:CD2	3:A3:204:VAL:HG11	2.38	0.54
5:AA:19:G:O2'	5:AA:477:G:N3	2.38	0.54
5:AA:699:C:N4	5:AA:700:G:O6	2.40	0.54
5:AA:1479:C:OP1	18:AN:127:ARG:NH2	2.40	0.54
3:B4:201:LEU:H	3:B4:201:LEU:HD12	1.73	0.54
5:BA:1152:C:OP1	7:BC:145:ARG:NH1	2.41	0.54
9:BE:24:ASP:OD1	9:BE:27:ARG:NH1	2.40	0.54
3:B4:255:GLU:N	3:B4:255:GLU:OE1	2.38	0.54
14:BJ:5:ASP:OD1	14:BJ:7:LEU:N	2.38	0.54
5:AA:31:U:O2	5:AA:501:G:C2	2.61	0.54
2:B2:19:ILE:O	2:B2:23:ILE:HG22	2.08	0.54
5:BA:743:U:O2'	5:BA:745:G:N7	2.31	0.54
8:BD:118:ARG:HB2	8:BD:191:LEU:HD21	1.90	0.54
18:BN:13:LYS:NZ	18:BN:74:LYS:O	2.36	0.54
5:AA:621:G:O2'	22:AR:117:HIS:ND1	2.40	0.54
10:AF:211:ASP:O	10:AF:227:LYS:N	2.41	0.54
23:AS:18:ASP:OD2	23:AS:21:CYS:N	2.40	0.54
26:AV:128:PHE:CE2	26:AV:132:ILE:HD11	2.42	0.54
3:B4:97:ILE:HG22	3:B4:98:GLU:OE1	2.07	0.54
5:BA:473:A:C5	5:BA:482:G:N2	2.76	0.54
5:BA:911:C:H5"	5:BA:923:A:H61	1.73	0.54
5:BA:1170:C:O2	5:BA:1174:A:O2'	2.25	0.54
9:BE:169:MET:SD	9:BE:169:MET:N	2.81	0.54
15:AK:35:THR:HG22	15:AK:95:ILE:HD12	1.90	0.53
27:AW:37:LYS:NZ	27:AW:51:THR:O	2.24	0.53
1:B1:22:GLU:OE2	1:B1:41:GLU:N	2.36	0.53
29:AY:35:VAL:O	29:AY:44:LEU:N	2.36	0.53
3:B3:10:VAL:HA	3:B3:199:ILE:HD11	1.90	0.53
3:B3:288:SER:O	3:B3:291:GLN:NE2	2.41	0.53
14:BJ:38:LEU:HD11	14:BJ:63:VAL:HG21	1.90	0.53
19:BO:136:GLU:O	19:BO:140:GLY:N	2.41	0.53
5:AA:207:G:N2	5:AA:210:A:OP2	2.37	0.53
9:AE:61:ALA:O	9:AE:62:ARG:NE	2.42	0.53
24:AT:29:GLU:OE1	24:AT:29:GLU:N	2.41	0.53
5:BA:1060:G:OP1	7:BC:154:VAL:HG22	2.07	0.53
3:A4:134:LEU:HD11	3:A4:278:LEU:HD21	1.91	0.53
5:AA:462:A:N1	9:AE:18:TRP:NE1	2.57	0.53
15:AK:67:ASP:OD1	15:AK:68:LYS:NZ	2.39	0.53
20:AP:15:LEU:HD21	20:AP:28:ILE:HG13	1.91	0.53
29:AY:48:THR:HG21	29:AY:53:ILE:HD11	1.90	0.53
26:BV:62:VAL:HG22	26:BV:68:VAL:HG11	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AA:581:G:O2'	9:AE:65:GLN:OE1	2.26	0.53
5:AA:1265:G:O2'	5:AA:1266:A:O5'	2.26	0.53
11:AG:33:ASP:OD2	11:AG:36:GLU:N	2.41	0.53
7:BC:64:GLU:OE2	7:BC:68:ILE:HD11	2.09	0.53
13:BI:86:MET:N	13:BI:86:MET:SD	2.81	0.53
17:BM:40:LEU:HD23	17:BM:41:PRO:O	2.08	0.53
5:AA:150:G:N3	12:AH:120:ASN:ND2	2.56	0.53
3:B4:266:ARG:NH2	3:B4:268:THR:O	2.41	0.53
5:BA:1026:A:H61	5:BA:1035:C:H42	1.54	0.53
5:BA:1209:C:O2	5:BA:1249:A:N6	2.41	0.53
10:BF:196:LYS:NZ	10:BF:242:LEU:O	2.39	0.53
7:AC:185:PRO:O	7:AC:188:ARG:NH2	2.42	0.53
23:BS:64:GLU:OE1	23:BS:66:ARG:NE	2.41	0.53
5:AA:11:A:N3	5:AA:1032:A:O2'	2.42	0.53
5:AA:257:U:OP1	15:AK:30:ARG:NH1	2.35	0.53
6:AB:21:THR:OG1	6:AB:22:GLN:N	2.42	0.53
3:B3:232:LEU:O	3:B3:235:LEU:HD23	2.09	0.53
5:BA:704:C:H5"	22:BR:78:ILE:HD12	1.89	0.53
3:A4:34:LEU:O	3:A4:37:THR:OG1	2.22	0.53
5:AA:1055:C:H5"	6:AB:97:LEU:HD22	1.90	0.53
11:AG:128:CYS:SG	11:AG:139:HIS:NE2	2.74	0.53
5:BA:6:G:O6	11:BG:192:ARG:NH2	2.42	0.53
5:BA:288:G:O2'	5:BA:561:A:N6	2.42	0.53
10:BF:165:LEU:HD12	10:BF:175:GLU:HB2	1.89	0.53
11:BG:135:CYS:SG	11:BG:137:ARG:NH1	2.82	0.53
11:AG:164:GLY:N	11:AG:182:ASP:OD1	2.39	0.52
12:AH:17:LYS:NZ	12:AH:50:LEU:O	2.35	0.52
19:AO:34:VAL:HG13	19:AO:35:LEU:CD2	2.35	0.52
19:AO:103:VAL:CG2	19:AO:105:ILE:HD11	2.38	0.52
5:BA:511:C:OP2	5:BA:512:U:O2'	2.17	0.52
1:A1:28:ILE:HD11	1:A1:34:GLU:N	2.24	0.52
5:AA:1076:G:O6	5:AA:1107:C:N4	2.41	0.52
5:AA:1281:U:H5	5:AA:1282:C:HO2'	1.57	0.52
7:AC:20:PHE:CZ	7:AC:68:ILE:HG21	2.45	0.52
12:AH:27:GLU:OE1	12:AH:27:GLU:N	2.41	0.52
13:AI:45:PRO:HB3	13:AI:64:VAL:HG13	1.90	0.52
5:BA:1061:A:OP2	7:BC:154:VAL:HG21	2.10	0.52
5:BA:1162:G:O2'	5:BA:1163:U:O4'	2.24	0.52
26:BV:83:ARG:HG3	26:BV:86:ALA:HB3	1.92	0.52
2:A2:17:LYS:NZ	5:AA:1466:G:N7	2.47	0.52
5:AA:730:G:H22	5:AA:756:A:P	2.32	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:AY:14:LEU:HB3	29:AY:58:ILE:HD13	1.90	0.52
5:BA:769:A:N3	5:BA:1482:C:O2'	2.32	0.52
5:BA:917:A:H62	25:BU:111:LYS:HE2	1.75	0.52
10:BF:204:ARG:NH1	10:BF:211:ASP:OD1	2.42	0.52
22:BR:49:MET:O	22:BR:52:THR:OG1	2.27	0.52
5:AA:835:C:O3'	14:AJ:76:LYS:NZ	2.25	0.52
19:AO:87:PHE:HB2	19:AO:122:ILE:HG21	1.91	0.52
6:BB:97:LEU:O	6:BB:100:THR:OG1	2.28	0.52
6:AB:169:TRP:NE1	6:AB:190:ILE:O	2.42	0.52
6:BB:68:LEU:HD23	6:BB:112:PRO:HB3	1.91	0.52
8:BD:119:VAL:HG22	8:BD:188:ILE:HG23	1.91	0.52
5:AA:1199:A:H4'	5:AA:1200:U:H2'	1.91	0.52
5:BA:442:C:OP1	27:BW:61:GLY:N	2.42	0.52
5:BA:533:C:H42	5:BA:715:C:H42	1.56	0.52
5:BA:1097:G:O2'	26:BV:6:ASP:OD2	2.28	0.52
5:AA:368:C:O2'	5:AA:369:A:OP2	2.23	0.52
23:BS:21:CYS:SG	23:BS:24:HIS:ND1	2.75	0.52
1:A1:16:ARG:NH2	11:AG:210:ARG:O	2.43	0.52
3:A3:114:GLU:OE2	3:A3:117:LYS:NZ	2.34	0.52
20:AP:30:GLY:O	20:AP:92:HIS:NE2	2.40	0.52
5:BA:114:A:N3	23:BS:28:LYS:NZ	2.58	0.52
26:AV:128:PHE:CZ	26:AV:132:ILE:HD11	2.45	0.52
5:BA:701:G:O2'	22:BR:55:ARG:NH2	2.43	0.52
8:BD:129:ILE:HD11	8:BD:178:TYR:CD1	2.45	0.52
10:BF:154:GLU:OE2	10:BF:154:GLU:N	2.42	0.52
5:AA:93:A:H62	5:AA:320:G:H21	1.57	0.52
6:AB:68:LEU:HD21	6:AB:110:PHE:CD2	2.44	0.52
6:AB:130:ALA:O	6:AB:134:GLY:N	2.41	0.52
22:AR:56:ASP:OD1	29:AY:35:VAL:HG22	2.09	0.52
5:BA:1314:C:H42	5:BA:1328:G:H1	1.58	0.52
11:BG:92:ARG:NH1	11:BG:176:ARG:O	2.43	0.52
17:BM:50:ARG:NE	17:BM:52:SER:OG	2.43	0.52
3:A3:104:ARG:NH1	3:A3:105:LYS:O	2.43	0.51
3:A3:192:TYR:O	3:A3:193:SER:OG	2.20	0.51
9:AE:52:ARG:NH2	11:AG:161:ARG:O	2.41	0.51
5:BA:139:C:N4	5:BA:153:G:O6	2.42	0.51
5:BA:431:U:O2'	5:BA:432:G:OP1	2.23	0.51
5:BA:1334:A:OP1	13:BI:97:LYS:NZ	2.43	0.51
18:BN:39:ILE:HD13	18:BN:76:ILE:HD11	1.92	0.51
20:BP:31:ILE:HD11	20:BP:66:LEU:HD22	1.92	0.51
5:AA:144:G:O2'	5:AA:340:A:N6	2.42	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AA:1029:G:O2'	5:AA:1031:G:O6	2.27	0.51
5:AA:1066:C:O2'	17:AM:67:ARG:NH2	2.42	0.51
5:BA:941:C:N4	5:BA:1183:C:N3	2.54	0.51
5:BA:1063:A:H61	7:BC:155:GLY:CA	2.23	0.51
20:BP:37:THR:CG2	26:BV:44:LEU:HD23	2.40	0.51
22:BR:24:ILE:HD12	22:BR:24:ILE:H	1.74	0.51
27:BW:4:ARG:O	27:BW:6:LYS:NZ	2.44	0.51
5:AA:640:U:HO2'	5:AA:641:A:C5'	2.22	0.51
30:AZ:28:LYS:HD2	30:AZ:40:VAL:HG12	1.92	0.51
4:B5:25:ILE:HB	4:B5:107:ALA:HB2	1.92	0.51
5:BA:1139:A:H4'	16:BL:108:VAL:HG13	1.92	0.51
7:BC:17:ILE:HD11	7:BC:75:LEU:HD11	1.92	0.51
14:BJ:38:LEU:HA	14:BJ:41:MET:SD	2.49	0.51
10:AF:139:GLN:OE1	10:AF:148:HIS:N	2.43	0.51
22:AR:67:LYS:HZ3	22:AR:72:PRO:HA	1.76	0.51
5:BA:1226:G:O6	26:BV:99:ARG:NH2	2.44	0.51
5:AA:507:G:OP1	19:AO:38:LYS:NZ	2.43	0.51
5:AA:1151:A:O3'	7:AC:153:LYS:NZ	2.44	0.51
9:AE:85:GLU:OE1	9:AE:85:GLU:N	2.43	0.51
27:AW:41:VAL:HA	27:AW:46:LEU:HD13	1.93	0.51
5:BA:143:G:H21	12:BH:71:GLY:HA3	1.76	0.51
11:BG:20:THR:HG23	11:BG:22:LEU:H	1.76	0.51
11:BG:25:MET:SD	11:BG:25:MET:N	2.80	0.51
11:BG:67:ASP:OD2	11:BG:194:THR:OG1	2.29	0.51
11:BG:160:PRO:HD2	11:BG:163:LEU:HD22	1.93	0.51
22:BR:137:LYS:NZ	22:BR:144:LYS:O	2.25	0.51
3:A4:272:GLU:OE1	3:A4:272:GLU:N	2.43	0.51
3:B3:60:LYS:NZ	3:B3:102:TYR:OH	2.39	0.51
4:B5:23:VAL:HG22	4:B5:52:ILE:HD13	1.92	0.51
10:BF:139:GLN:OE1	10:BF:140:LEU:N	2.44	0.51
10:BF:180:GLU:N	10:BF:180:GLU:OE1	2.43	0.51
5:AA:181:G:H21	23:AS:6:GLY:C	2.14	0.51
5:AA:483:G:OP2	5:AA:483:G:N2	2.35	0.51
14:AJ:49:GLU:OE1	14:AJ:49:GLU:N	2.37	0.51
5:BA:144:G:N2	5:BA:147:A:OP2	2.42	0.51
5:BA:1256:C:O2'	5:BA:1262:U:N3	2.43	0.51
5:BA:1485:G:N2	5:BA:1486:A:N1	2.58	0.51
16:BL:47:GLU:OE2	16:BL:102:TYR:OH	2.16	0.51
5:AA:96:G:H21	5:AA:350:G:C4'	2.24	0.51
5:AA:463:G:H1'	5:AA:495:G:H21	1.74	0.51
5:AA:615:G:C6	5:AA:698:A:N1	2.79	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AA:1243:C:OP1	26:AV:72:ARG:NH2	2.42	0.51
20:AP:95:THR:OG1	20:AP:96:ALA:N	2.44	0.51
4:A5:19:ALA:HB2	4:A5:78:ILE:HD13	1.93	0.51
5:AA:1184:U:OP1	20:AP:130:ARG:NH2	2.44	0.51
9:AE:89:LEU:O	9:AE:92:VAL:HG22	2.10	0.51
10:AF:110:LEU:HD12	10:AF:110:LEU:O	2.11	0.51
12:AH:34:ILE:HD11	12:AH:74:MET:HB2	1.92	0.51
19:AO:93:ALA:O	19:AO:97:ILE:HD12	2.10	0.51
20:AP:55:THR:OG1	20:AP:58:GLN:OE1	2.27	0.51
26:AV:16:VAL:HG22	26:AV:132:ILE:HD13	1.93	0.51
5:BA:91:G:OP1	5:BA:321:A:N6	2.43	0.51
5:BA:684:G:O2'	5:BA:720:A:O4'	2.25	0.51
5:BA:1479:C:OP1	18:BN:127:ARG:NH2	2.44	0.51
13:BI:104:VAL:HG12	13:BI:108:PHE:CZ	2.45	0.51
5:AA:136:A:N7	5:AA:155:U:C2	2.78	0.51
5:AA:529:C:O2'	5:AA:530:G:O5'	2.22	0.51
5:BA:937:A:C2	5:BA:1276:G:N2	2.77	0.51
15:BK:35:THR:O	15:BK:95:ILE:HD12	2.11	0.51
3:A3:94:VAL:O	3:A4:2:LYS:NZ	2.37	0.50
3:A4:131:GLY:HA2	3:A4:134:LEU:HD12	1.93	0.50
5:AA:1047:U:P	5:AA:1060:G:H22	2.33	0.50
5:BA:302:A:H61	9:BE:6:ARG:HH12	1.59	0.50
9:BE:12:GLU:OE2	9:BE:49:LYS:NZ	2.24	0.50
13:BI:176:ASN:OD1	13:BI:177:LYS:N	2.44	0.50
20:BP:20:GLN:O	20:BP:24:ALA:N	2.44	0.50
29:BY:48:THR:OG1	29:BY:51:LYS:O	2.28	0.50
5:AA:1069:G:N2	5:AA:1140:A:N3	2.58	0.50
3:B3:109:ALA:O	3:B3:110:SER:OG	2.18	0.50
5:BA:381:C:N4	5:BA:382:G:O6	2.44	0.50
13:BI:25:ASP:OD2	13:BI:118:ASN:ND2	2.44	0.50
22:BR:109:LEU:HD13	22:BR:119:MET:CE	2.41	0.50
5:AA:56:A:N6	5:AA:91:G:O2'	2.45	0.50
5:AA:706:G:H5'	22:AR:139:LYS:HZ1	1.75	0.50
6:AB:62:PHE:HB2	6:AB:67:ILE:HD11	1.94	0.50
25:AU:22:GLU:OE1	25:AU:22:GLU:N	2.44	0.50
4:B5:15:LEU:HG	4:B5:78:ILE:HD11	1.94	0.50
5:BA:772:G:N2	5:BA:774:U:HO2'	2.09	0.50
5:BA:1107:C:O2'	16:BL:7:THR:HG22	2.12	0.50
11:BG:145:VAL:HG11	11:BG:208:THR:HG22	1.94	0.50
6:BB:44:ASP:OD1	6:BB:46:ARG:NE	2.43	0.50
26:BV:102:LEU:HD13	26:BV:119:ARG:HD2	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AA:1096:G:O3'	16:AL:25:ARG:NH1	2.45	0.50
20:AP:83:LYS:N	20:AP:90:ASP:OD1	2.43	0.50
4:B5:94:VAL:HG11	5:BA:959:G:H2'	1.93	0.50
6:BB:131:VAL:HG21	6:BB:149:TYR:CE1	2.47	0.50
20:BP:115:TYR:OH	20:BP:119:ARG:NH1	2.45	0.50
30:BZ:33:GLU:N	30:BZ:33:GLU:OE1	2.45	0.50
3:A3:108:LEU:HG	3:A3:112:LEU:HD13	1.94	0.50
5:AA:366:C:O2'	5:AA:435:A:N1	2.40	0.50
5:AA:431:U:O2'	5:AA:432:G:OP1	2.23	0.50
6:AB:145:ASN:OD1	6:AB:158:ASN:ND2	2.40	0.50
9:AE:42:TRP:O	9:AE:46:THR:OG1	2.28	0.50
13:AI:82:ALA:HB3	13:AI:84:HIS:CE1	2.47	0.50
13:AI:115:THR:O	13:AI:117:LYS:NZ	2.44	0.50
19:AO:30:TYR:O	19:AO:34:VAL:HG12	2.12	0.50
22:AR:90:GLU:N	22:AR:90:GLU:OE2	2.44	0.50
5:BA:813:G:OP2	5:BA:829:U:N3	2.44	0.50
20:BP:60:LYS:HE3	20:BP:60:LYS:HA	1.94	0.50
22:BR:109:LEU:HD13	22:BR:119:MET:HE2	1.94	0.50
29:BY:17:LYS:HB2	29:BY:59:LEU:HD11	1.93	0.50
3:A3:92:LEU:HD23	3:A3:104:ARG:O	2.12	0.50
17:AM:10:SER:OG	17:AM:93:ASP:OD2	2.30	0.50
23:AS:51:ARG:N	23:AS:68:SER:O	2.40	0.50
25:AU:24:LEU:HD21	25:AU:74:PRO:CD	2.42	0.50
5:BA:807:C:OP1	6:BB:24:LYS:NZ	2.40	0.50
5:BA:1283:G:O6	25:BU:31:ARG:NH1	2.40	0.50
13:BI:76:GLY:N	13:BI:86:MET:O	2.45	0.50
13:BI:104:VAL:HG12	13:BI:108:PHE:CE2	2.47	0.50
2:A2:34:ARG:NH1	5:AA:851:C:OP1	2.45	0.50
5:AA:56:A:N6	5:AA:91:G:HO2'	2.10	0.50
23:AS:91:THR:HG22	23:AS:92:ARG:H	1.77	0.50
25:AU:24:LEU:HD11	25:AU:74:PRO:HG2	1.93	0.50
5:BA:559:G:H21	5:BA:587:G:H21	1.60	0.50
5:BA:1274:C:OP2	25:BU:34:ARG:NE	2.45	0.50
8:BD:119:VAL:HG13	8:BD:188:ILE:HG12	1.93	0.50
19:BO:77:LEU:HD21	19:BO:80:ASN:OD1	2.10	0.50
3:A3:213:TYR:CE2	3:A3:232:LEU:HD13	2.47	0.50
5:AA:7:G:N7	11:AG:192:ARG:NH1	2.60	0.50
13:AI:187:GLU:OE2	13:AI:199:TYR:N	2.45	0.50
5:BA:165:U:O2	5:BA:198:A:N6	2.45	0.50
5:BA:1306:A:H61	5:BA:1334:A:H3'	1.77	0.50
8:BD:122:MET:N	8:BD:122:MET:SD	2.84	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:BG:143:PHE:O	11:BG:145:VAL:HG13	2.11	0.50
5:AA:14:C:OP1	11:AG:151:SER:OG	2.20	0.49
5:AA:91:G:H3'	5:AA:92:G:H21	1.77	0.49
7:AC:31:GLY:HA3	7:AC:85:ILE:HD11	1.94	0.49
12:AH:81:PRO:O	12:AH:108:ARG:NE	2.40	0.49
5:BA:260:C:O3'	23:BS:92:ARG:NH2	2.45	0.49
5:BA:530:G:H22	5:BA:718:G:N2	2.09	0.49
8:BD:112:LYS:O	8:BD:112:LYS:NZ	2.30	0.49
11:BG:56:GLU:OE2	11:BG:227:ARG:NH2	2.45	0.49
12:BH:45:ILE:HD11	12:BH:50:LEU:HD21	1.93	0.49
14:BJ:48:GLY:N	14:BJ:66:LEU:HD11	2.27	0.49
23:BS:45:LYS:O	23:BS:98:LYS:NZ	2.45	0.49
27:BW:33:ARG:NH1	27:BW:53:ILE:O	2.45	0.49
5:AA:960:A:O4'	5:AA:988:A:N6	2.45	0.49
25:AU:94:ILE:HG23	25:AU:98:MET:HG3	1.94	0.49
27:AW:53:ILE:HG23	27:AW:69:ALA:HB2	1.94	0.49
29:AY:16:VAL:HG12	29:AY:58:ILE:HA	1.94	0.49
5:BA:1201:G:OP1	13:BI:91:ARG:NH1	2.44	0.49
5:BA:1243:C:OP1	26:BV:72:ARG:NH2	2.40	0.49
6:BB:68:LEU:O	6:BB:115:LEU:HD12	2.11	0.49
7:BC:161:LEU:HD13	7:BC:187:ALA:HB1	1.93	0.49
13:BI:189:ILE:O	13:BI:193:ASN:ND2	2.46	0.49
3:A4:116:PHE:CE1	3:A4:277:LEU:HD22	2.47	0.49
5:AA:1079:G:H21	5:AA:1106:A:H62	1.59	0.49
6:AB:138:VAL:HG13	6:AB:152:LEU:HG	1.94	0.49
25:AU:85:ASN:ND2	25:AU:88:GLU:OE2	2.45	0.49
5:BA:918:A:N6	25:BU:109:THR:O	2.45	0.49
8:BD:124:ILE:O	8:BD:181:ARG:N	2.44	0.49
9:BE:160:PHE:O	9:BE:168:ARG:NH1	2.43	0.49
10:BF:134:LYS:O	10:BF:137:ARG:NH1	2.46	0.49
11:BG:51:ASP:N	11:BG:51:ASP:OD1	2.45	0.49
11:BG:64:GLU:O	11:BG:88:ALA:N	2.42	0.49
3:A3:166:ASP:OD1	3:A3:167:GLN:N	2.46	0.49
4:A5:65:HIS:HB2	28:AX:10:ILE:HD12	1.93	0.49
5:AA:64:G:H22	5:AA:85:A:H2	1.60	0.49
6:AB:23:GLN:NE2	6:AB:24:LYS:O	2.45	0.49
16:AL:46:LEU:HD23	16:AL:50:ILE:HD11	1.94	0.49
20:AP:113:ARG:HD2	20:AP:118:ILE:HD11	1.95	0.49
26:AV:61:ARG:HH12	26:AV:64:LEU:HD12	1.76	0.49
5:BA:968:C:N3	28:BX:37:ARG:NH2	2.60	0.49
7:BC:2:ALA:HB3	7:BC:5:ARG:HB2	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:BD:117:LEU:HD13	8:BD:190:VAL:HA	1.94	0.49
9:BE:82:LEU:HB3	9:BE:83:LEU:HD22	1.95	0.49
23:BS:61:GLU:OE1	23:BS:61:GLU:N	2.45	0.49
5:AA:237:C:P	19:AO:21:LYS:HZ2	2.35	0.49
5:AA:1276:G:O6	25:AU:31:ARG:NH2	2.46	0.49
6:AB:21:THR:O	6:AB:41:TYR:N	2.40	0.49
20:AP:94:ILE:HG12	20:AP:95:THR:HG23	1.93	0.49
5:BA:14:C:OP1	11:BG:151:SER:OG	2.29	0.49
11:BG:166:VAL:O	11:BG:185:SER:OG	2.19	0.49
13:BI:40:GLU:OE2	13:BI:42:ARG:NE	2.41	0.49
5:AA:320:G:N7	15:AK:47:ARG:NH1	2.60	0.49
13:AI:87:ARG:NE	13:AI:88:ARG:O	2.38	0.49
18:AN:61:MET:HB2	18:AN:104:ALA:HB2	1.93	0.49
21:AQ:38:LEU:HD12	21:AQ:39:CYS:H	1.78	0.49
1:B1:40:CYS:O	1:B1:44:ARG:N	2.45	0.49
3:B3:33:LYS:O	3:B3:37:THR:OG1	2.19	0.49
5:BA:1016:G:O2'	5:BA:1150:G:N2	2.45	0.49
11:BG:24:MET:SD	11:BG:24:MET:N	2.77	0.49
3:A4:35:VAL:HB	3:A4:82:ILE:HD11	1.94	0.49
3:A4:174:ILE:O	3:A4:177:SER:OG	2.26	0.49
4:A5:59:PRO:HG2	4:A5:62:ILE:HD12	1.94	0.49
5:AA:885:G:O2'	5:AA:1458:A:N6	2.45	0.49
18:AN:61:MET:SD	18:AN:62:LEU:N	2.86	0.49
3:B4:107:LYS:N	3:B4:292:ASP:OD2	2.45	0.49
5:BA:1029:G:O2'	5:BA:1031:G:O6	2.30	0.49
5:BA:1211:A:HO2'	5:BA:1329:C:HO2'	1.61	0.49
8:BD:141:MET:CE	8:BD:170:ILE:HD12	2.43	0.49
8:BD:156:ASP:OD1	8:BD:157:PHE:N	2.46	0.49
14:BJ:118:GLU:OE1	14:BJ:119:LYS:N	2.46	0.49
5:AA:627:G:O3'	8:AD:118:ARG:NH1	2.45	0.49
5:AA:1118:C:OP2	24:AT:49:ARG:NH2	2.46	0.49
8:AD:113:ASP:OD1	8:AD:113:ASP:N	2.45	0.49
11:AG:67:ASP:N	11:AG:67:ASP:OD1	2.43	0.49
13:AI:48:HIS:O	16:AL:112:ARG:NH2	2.40	0.49
20:AP:14:ASP:O	20:AP:15:LEU:HD23	2.12	0.49
5:BA:937:A:OP1	5:BA:939:C:N4	2.46	0.49
5:BA:1076:G:HO2'	5:BA:1077:U:P	2.36	0.49
7:BC:20:PHE:CZ	7:BC:68:ILE:HG21	2.47	0.49
13:BI:31:PRO:O	13:BI:34:LYS:NZ	2.42	0.49
5:AA:1477:U:H2'	5:AA:1478:A:H8	1.78	0.49
4:B5:11:VAL:HG13	4:B5:15:LEU:HD23	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:BD:17:GLN:OE1	8:BD:17:GLN:N	2.46	0.49
5:AA:511:C:OP2	5:AA:512:U:O2'	2.20	0.49
5:AA:655:A:O3'	3:B4:10:VAL:HG21	2.13	0.49
6:AB:156:THR:OG1	6:AB:157:ASN:N	2.46	0.49
5:BA:94:C:OP1	10:BF:4:LYS:N	2.40	0.49
10:BF:45:LEU:HD21	10:BF:81:TYR:HA	1.95	0.49
17:BM:66:LEU:HD21	21:BQ:52:PHE:CD1	2.48	0.49
27:BW:44:LEU:HB3	27:BW:46:LEU:HD21	1.95	0.49
3:A4:157:LYS:NZ	3:A4:187:GLU:OE1	2.46	0.48
5:AA:111:G:HO2'	5:AA:112:G:P	2.35	0.48
5:AA:557:G:N1	5:AA:589:U:N3	2.61	0.48
14:AJ:22:LYS:O	14:AJ:65:LEU:HD13	2.13	0.48
5:BA:351:C:O2'	5:BA:384:G:N3	2.44	0.48
5:BA:358:G:O2'	5:BA:360:A:N6	2.19	0.48
6:BB:27:ASP:OD1	6:BB:28:MET:N	2.46	0.48
5:AA:33:U:N3	5:AA:393:A:O4'	2.41	0.48
5:AA:274:G:OP2	23:AS:69:LYS:NZ	2.46	0.48
5:AA:334:G:O6	5:AA:346:C:N4	2.46	0.48
5:AA:967:C:O2'	5:AA:968:C:O4'	2.19	0.48
5:AA:1332:C:OP2	16:AL:11:LYS:NZ	2.44	0.48
15:AK:107:LYS:HB3	15:AK:125:LEU:HD12	1.95	0.48
3:B3:126:LYS:HA	3:B3:129:LEU:HD12	1.95	0.48
5:BA:1043:U:H1'	24:BT:4:ILE:HD11	1.94	0.48
5:BA:1264:G:N2	5:BA:1293:A:H62	2.05	0.48
4:A5:6:TYR:OH	4:A5:54:ALA:O	2.32	0.48
13:AI:76:GLY:N	13:AI:86:MET:O	2.36	0.48
10:BF:127:ILE:O	10:BF:161:SER:N	2.36	0.48
22:BR:105:LEU:CD1	22:BR:109:LEU:HD21	2.43	0.48
27:BW:47:ASN:O	27:BW:51:THR:HG23	2.13	0.48
5:AA:16:G:H21	5:AA:872:A:H62	1.61	0.48
3:B3:14:GLN:O	3:B3:17:LYS:NZ	2.43	0.48
5:BA:559:G:H21	5:BA:587:G:N2	2.11	0.48
5:BA:892:C:N4	5:BA:896:A:H61	2.12	0.48
7:BC:189:LEU:N	7:BC:192:GLU:OE1	2.45	0.48
11:BG:5:TRP:CZ2	11:BG:59:ALA:HB2	2.43	0.48
17:BM:54:ASP:N	17:BM:54:ASP:OD1	2.46	0.48
30:BZ:13:GLU:O	30:BZ:28:LYS:N	2.44	0.48
3:A3:217:LYS:NZ	3:A3:219:GLU:O	2.46	0.48
4:A5:27:ARG:NH2	4:A5:28:ASP:OD1	2.46	0.48
5:AA:419:G:N2	9:AE:167:GLU:OE2	2.40	0.48
5:AA:968:C:N3	28:AX:37:ARG:NH2	2.61	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:AO:39:GLU:OE1	19:AO:39:GLU:N	2.42	0.48
5:BA:334:G:H22	5:BA:347:G:H1	1.61	0.48
5:BA:849:U:OP2	5:BA:864:G:N1	2.39	0.48
16:BL:25:ARG:N	16:BL:61:ASP:OD1	2.46	0.48
29:BY:11:SER:HG	29:BY:28:PHE:HZ	1.59	0.48
4:A5:23:VAL:HG22	4:A5:52:ILE:HD13	1.94	0.48
5:AA:866:A:OP1	19:AO:31:LYS:NZ	2.25	0.48
9:AE:30:MET:HB3	9:AE:41:LEU:HD11	1.96	0.48
5:BA:726:A:N6	5:BA:762:G:O6	2.46	0.48
7:BC:15:MET:HE3	21:BQ:50:LEU:N	2.28	0.48
3:A4:135:VAL:O	3:A4:137:THR:N	2.47	0.48
5:AA:706:G:C5'	22:AR:139:LYS:HZ1	2.26	0.48
5:AA:1296:U:O2'	13:AI:85:PHE:O	2.31	0.48
5:AA:1365:G:O2'	5:AA:1473:A:O2'	1.99	0.48
10:AF:167:LYS:HB2	10:AF:174:LEU:HD21	1.96	0.48
5:BA:1472:G:H2'	5:BA:1473:A:C8	2.48	0.48
15:BK:66:PHE:O	15:BK:123:ILE:HD12	2.14	0.48
22:BR:151:GLU:OE1	22:BR:151:GLU:N	2.45	0.48
5:AA:557:G:C6	5:AA:589:U:N3	2.80	0.48
5:AA:684:G:N2	5:AA:719:G:O3'	2.44	0.48
5:AA:1180:G:N2	25:AU:86:GLY:O	2.47	0.48
5:AA:1210:A:OP1	16:AL:68:GLY:N	2.45	0.48
5:AA:1267:U:OP1	20:AP:129:GLN:NE2	2.47	0.48
14:AJ:81:VAL:HG12	14:AJ:82:LYS:O	2.14	0.48
23:AS:35:GLU:OE1	23:AS:35:GLU:N	2.47	0.48
23:AS:60:TYR:O	23:AS:62:ARG:NE	2.47	0.48
27:AW:87:LEU:HD22	27:AW:93:ILE:HD12	1.95	0.48
5:BA:1165:U:HO2'	5:BA:1166:G:H8	1.61	0.48
5:BA:1185:A:OP1	20:BP:131:THR:N	2.43	0.48
5:BA:1341:C:O2'	5:BA:1342:C:O5'	2.31	0.48
10:BF:202:ILE:HG12	10:BF:213:VAL:HG12	1.94	0.48
3:A3:231:GLU:O	3:A3:235:LEU:HD22	2.14	0.48
5:BA:540:G:N1	5:BA:708:C:OP2	2.42	0.48
7:BC:58:GLY:O	7:BC:63:ARG:NH2	2.45	0.48
11:BG:67:ASP:OD1	11:BG:68:ILE:N	2.46	0.48
22:BR:126:GLU:OE1	22:BR:127:SER:N	2.47	0.48
29:BY:36:ARG:NE	29:BY:41:GLY:O	2.47	0.48
5:AA:1112:G:OP1	17:AM:69:HIS:ND1	2.47	0.48
5:AA:1119:U:OP1	24:AT:5:ARG:NH1	2.42	0.48
13:AI:179:SER:N	13:AI:182:GLU:OE1	2.41	0.48
19:AO:10:GLU:O	23:AS:63:TYR:N	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:AW:78:MET:CE	27:AW:92:LEU:HD13	2.44	0.48
5:BA:968:C:O2	28:BX:37:ARG:NH1	2.46	0.48
5:BA:1098:G:H1'	26:BV:3:THR:HG21	1.95	0.48
5:BA:1105:C:O2'	5:BA:1106:A:O5'	2.27	0.48
5:BA:1196:A:OP1	26:BV:82:ASN:ND2	2.42	0.48
15:BK:39:GLU:OE2	15:BK:40:GLN:NE2	2.46	0.48
20:BP:29:LYS:HG3	20:BP:95:THR:HG22	1.94	0.48
27:BW:28:GLU:OE1	27:BW:28:GLU:N	2.46	0.48
3:A3:97:ILE:HG12	3:A4:3:VAL:HG21	1.96	0.47
7:AC:4:GLU:O	7:AC:8:ILE:HG22	2.14	0.47
10:AF:228:GLU:OE1	10:AF:228:GLU:N	2.45	0.47
30:AZ:32:LEU:HD13	30:AZ:37:LYS:HZ3	1.79	0.47
23:BS:87:LEU:HB3	23:BS:106:LEU:HD11	1.96	0.47
3:A3:19:LEU:HD21	3:A3:125:LEU:HG	1.96	0.47
3:A3:268:THR:OG1	3:A3:272:GLU:OE2	2.32	0.47
5:AA:1318:U:H5'	21:AQ:31:ILE:HD12	1.96	0.47
3:B3:187:GLU:O	3:B3:190:GLN:NE2	2.47	0.47
5:BA:176:U:O4	5:BA:187:C:C4	2.67	0.47
6:BB:70:VAL:HG22	6:BB:92:ILE:HB	1.96	0.47
16:BL:5:GLN:HG2	16:BL:18:VAL:HG12	1.95	0.47
5:AA:43:A:O2'	5:AA:44:C:OP2	2.30	0.47
6:AB:6:LEU:O	6:AB:173:ARG:NH2	2.42	0.47
18:AN:81:ILE:HD13	18:AN:102:ILE:HG12	1.96	0.47
23:AS:51:ARG:HE	23:AS:52:GLN:H	1.62	0.47
24:AT:25:THR:O	24:AT:31:ASN:ND2	2.39	0.47
5:BA:568:C:OP1	9:BE:79:ARG:NH1	2.43	0.47
5:BA:1207:G:OP2	26:BV:76:TYR:OH	2.31	0.47
27:BW:18:GLU:OE1	27:BW:18:GLU:N	2.46	0.47
5:AA:143:G:N1	5:AA:149:U:C2	2.82	0.47
6:AB:21:THR:HG22	6:AB:143:THR:HG23	1.95	0.47
19:AO:103:VAL:HG12	19:AO:129:VAL:HG23	1.96	0.47
5:BA:916:U:N3	5:BA:919:U:OP2	2.47	0.47
5:BA:1025:U:OP2	11:BG:112:LYS:NZ	2.20	0.47
5:BA:1310:C:N3	13:BI:95:SER:OG	2.46	0.47
5:BA:1328:G:N7	16:BL:122:SER:OG	2.35	0.47
9:BE:143:LEU:O	9:BE:143:LEU:HD23	2.14	0.47
20:BP:31:ILE:HD11	20:BP:66:LEU:CD2	2.44	0.47
5:AA:226:G:O3'	10:AF:7:LYS:NZ	2.47	0.47
5:AA:1459:G:OP1	5:AA:1462:A:O2'	2.22	0.47
9:AE:77:LEU:HB3	9:AE:83:LEU:HD12	1.96	0.47
12:AH:63:ILE:HD13	12:AH:121:VAL:CG1	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B3:160:ILE:O	3:B3:164:LEU:HD23	2.14	0.47
3:B3:165:SER:O	3:B3:167:GLN:NE2	2.48	0.47
5:BA:885:G:O2'	5:BA:1487:U:O4'	2.33	0.47
6:BB:60:ALA:HB3	6:BB:178:ASN:OD1	2.14	0.47
5:AA:245:U:O3'	15:AK:10:LYS:NZ	2.34	0.47
5:AA:1173:A:OP2	5:AA:1175:C:N4	2.48	0.47
23:AS:51:ARG:HE	23:AS:52:GLN:N	2.12	0.47
2:B2:23:ILE:HD11	5:BA:849:U:H5'	1.96	0.47
5:BA:936:A:N6	5:BA:1184:U:O4'	2.48	0.47
5:BA:1096:G:O3'	16:BL:25:ARG:NH1	2.48	0.47
14:BJ:114:LYS:HA	14:BJ:117:ILE:HD12	1.95	0.47
5:AA:71:C:H2'	5:AA:72:C:C1'	2.44	0.47
5:AA:896:A:O4'	5:AA:1341:C:N4	2.46	0.47
5:AA:1337:A:N6	13:AI:52:ALA:O	2.47	0.47
11:AG:95:TYR:HB3	11:AG:121:ILE:HD11	1.97	0.47
17:AM:8:ILE:HG22	17:AM:96:ILE:HG12	1.97	0.47
20:AP:10:VAL:HG22	20:AP:59:VAL:HG13	1.97	0.47
5:BA:257:U:OP2	15:BK:116:GLN:NE2	2.43	0.47
5:BA:672:G:HO2'	5:BA:673:C:P	2.35	0.47
8:BD:122:MET:SD	8:BD:186:ARG:NE	2.80	0.47
11:BG:218:ILE:HG23	11:BG:223:ILE:HB	1.95	0.47
5:AA:332:C:O2'	5:AA:1424:G:O4'	2.33	0.47
5:AA:474:G:N7	19:AO:70:ARG:NH1	2.63	0.47
5:AA:974:G:OP2	25:AU:64:ARG:NH1	2.48	0.47
5:AA:1238:G:HO2'	7:AC:2:ALA:N	2.12	0.47
3:B4:130:LEU:HD11	3:B4:278:LEU:HD21	1.97	0.47
5:BA:557:G:C6	5:BA:589:U:N3	2.83	0.47
5:BA:1162:G:H22	21:BQ:41:HIS:HB2	1.79	0.47
9:AE:59:LEU:HD13	11:AG:132:GLU:O	2.15	0.47
10:AF:45:LEU:HA	10:AF:48:ILE:HD12	1.97	0.47
24:AT:13:ALA:HB1	24:AT:57:LEU:HD11	1.96	0.47
29:AY:15:ARG:HB2	29:AY:62:LEU:HD11	1.97	0.47
2:B2:21:LYS:NZ	5:BA:1470:G:N7	2.63	0.47
3:B3:64:ASN:N	3:B3:64:ASN:OD1	2.48	0.47
5:BA:252:U:P	23:BS:45:LYS:HZ2	2.38	0.47
5:BA:1031:G:O2'	5:BA:1032:A:O5'	2.33	0.47
5:BA:1273:G:OP2	25:BU:33:ARG:NH2	2.48	0.47
11:BG:128:CYS:SG	11:BG:139:HIS:NE2	2.81	0.47
15:BK:86:ASN:OD1	15:BK:87:ARG:N	2.48	0.47
5:AA:331:C:OP1	12:AH:85:ARG:NH1	2.48	0.47
5:AA:957:A:N1	5:AA:991:C:N4	2.64	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:AS:20:LYS:HE2	23:AS:94:LEU:HD13	1.97	0.47
5:BA:675:A:N3	5:BA:676:G:N1	2.63	0.47
29:BY:13:PHE:C	29:BY:14:LEU:HD22	2.34	0.47
5:AA:111:G:N2	23:AS:90:GLU:OE2	2.48	0.46
10:AF:19:TRP:NE1	10:AF:42:SER:O	2.42	0.46
11:AG:20:THR:HG23	11:AG:23:GLY:H	1.80	0.46
23:AS:21:CYS:SG	23:AS:24:HIS:ND1	2.73	0.46
3:B3:215:ASP:OD1	3:B3:215:ASP:N	2.48	0.46
5:BA:1063:A:H61	7:BC:155:GLY:HA3	1.80	0.46
9:BE:83:LEU:CD1	9:BE:95:LEU:HD21	2.44	0.46
11:BG:140:SER:HA	11:BG:180:VAL:HG13	1.95	0.46
23:BS:108:ARG:N	23:BS:111:GLU:OE2	2.46	0.46
5:AA:535:U:H3	5:AA:713:A:H62	1.63	0.46
5:AA:726:A:N6	5:AA:762:G:O6	2.48	0.46
5:AA:1370:U:H3	5:AA:1445:A:H61	1.62	0.46
6:AB:44:ASP:OD1	6:AB:46:ARG:NH1	2.48	0.46
18:AN:103:ARG:NH2	30:AZ:61:GLU:OE2	2.47	0.46
3:B3:214:LEU:HD21	3:B3:225:VAL:HG13	1.96	0.46
5:BA:1030:U:O2	11:BG:196:ASN:ND2	2.48	0.46
23:BS:21:CYS:SG	23:BS:24:HIS:N	2.88	0.46
3:A3:218:ARG:O	3:A3:218:ARG:NH1	2.44	0.46
5:AA:315:A:H4'	5:AA:1422:G:H4'	1.97	0.46
5:AA:1252:C:H4'	13:AI:5:LEU:HD11	1.96	0.46
6:AB:103:ASN:O	6:AB:106:VAL:HG22	2.15	0.46
5:BA:462:A:N3	5:BA:496:C:O2'	2.44	0.46
3:A4:70:SER:O	3:A4:72:SER:N	2.49	0.46
5:AA:16:G:C4'	5:AA:526:A:H61	2.29	0.46
5:AA:1402:C:O2'	12:AH:79:HIS:NE2	2.43	0.46
8:AD:158:VAL:O	8:AD:161:SER:OG	2.27	0.46
5:BA:950:C:N4	5:BA:1173:A:H62	2.13	0.46
5:BA:1127:A:O2'	5:BA:1128:U:O2	2.23	0.46
9:BE:91:ASP:O	9:BE:94:SER:OG	2.31	0.46
21:BQ:37:MET:N	21:BQ:37:MET:SD	2.89	0.46
3:A4:294:GLN:OE1	3:A4:295:ASN:N	2.49	0.46
8:AD:156:ASP:OD1	8:AD:157:PHE:N	2.49	0.46
3:B3:54:ILE:HD12	3:B3:54:ILE:H	1.80	0.46
5:BA:145:A:N6	5:BA:340:A:N1	2.64	0.46
5:BA:1082:A:H4'	16:BL:18:VAL:HG21	1.98	0.46
5:AA:16:G:H4'	5:AA:526:A:H61	1.80	0.46
4:B5:69:LEU:HB2	28:BX:10:ILE:HD11	1.98	0.46
9:BE:73:LEU:HD23	9:BE:89:LEU:HD11	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:BI:151:ASP:OD1	13:BI:152:ILE:N	2.48	0.46
7:AC:166:TYR:OH	7:AC:168:GLN:OE1	2.33	0.46
17:AM:1:MET:SD	17:AM:2:GLN:N	2.89	0.46
22:AR:37:VAL:HG21	22:AR:81:ILE:HG21	1.96	0.46
23:AS:5:ILE:HG23	23:AS:7:LEU:H	1.80	0.46
29:AY:19:ILE:HD11	29:AY:56:ALA:HA	1.97	0.46
22:BR:95:LEU:HD23	22:BR:99:ILE:HD11	1.97	0.46
3:A4:61:ILE:HD11	3:A4:103:VAL:HB	1.96	0.46
5:AA:930:G:N2	5:AA:1323:A:OP2	2.46	0.46
5:AA:1140:A:OP1	16:AL:104:ARG:NH1	2.46	0.46
5:BA:1423:A:O2'	5:BA:1424:G:OP1	2.34	0.46
9:BE:21:GLU:OE2	9:BE:21:GLU:N	2.36	0.46
25:BU:72:ILE:HG21	25:BU:98:MET:HG3	1.98	0.46
3:A3:119:LEU:HD21	3:A3:123:GLU:HB3	1.98	0.46
5:AA:530:G:H22	5:AA:719:G:H1'	1.80	0.46
5:AA:824:G:O2'	5:AA:877:A:OP1	2.33	0.46
10:AF:96:THR:HG22	27:AW:12:LYS:HB2	1.98	0.46
14:AJ:45:GLY:O	14:AJ:66:LEU:HD12	2.15	0.46
18:AN:115:VAL:N	18:AN:116:GLU:OE2	2.49	0.46
2:B2:9:LYS:O	2:B2:13:ARG:NH2	2.47	0.46
7:BC:90:LEU:HD22	7:BC:184:PRO:HB3	1.97	0.46
12:BH:20:GLU:OE2	12:BH:22:THR:OG1	2.34	0.46
25:BU:114:GLU:OE1	25:BU:114:GLU:N	2.41	0.46
5:AA:963:A:H62	5:AA:988:A:H1'	1.81	0.46
5:BA:406:U:H3	5:BA:416:A:H61	1.63	0.46
5:BA:950:C:H42	5:BA:1173:A:H62	1.64	0.46
5:BA:1031:G:O2'	5:BA:1032:A:O4'	2.32	0.46
9:BE:150:ASP:OD1	9:BE:151:THR:HG23	2.16	0.46
1:A1:32:CYS:SG	1:A1:54:ASN:ND2	2.81	0.45
4:A5:78:ILE:HD12	4:A5:114:ILE:HG23	1.98	0.45
5:AA:228:G:O2'	5:AA:258:A:N1	2.42	0.45
7:AC:30:TYR:O	7:AC:93:LYS:NZ	2.37	0.45
5:BA:926:C:P	5:BA:927:A:HO2'	2.35	0.45
2:A2:24:ARG:NH2	5:AA:861:G:OP1	2.46	0.45
5:AA:568:C:OP1	9:AE:79:ARG:NH1	2.49	0.45
5:AA:702:G:OP1	22:AR:16:ARG:NH1	2.50	0.45
27:AW:11:ASN:O	27:AW:15:GLY:N	2.50	0.45
3:B3:151:GLU:OE1	3:B3:151:GLU:N	2.49	0.45
5:BA:646:U:OP2	18:BN:24:ASN:ND2	2.45	0.45
5:BA:918:A:O2'	5:BA:920:U:OP2	2.24	0.45
9:BE:30:MET:O	9:BE:34:GLU:N	2.41	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:BF:217:ASP:OD1	10:BF:218:GLU:N	2.43	0.45
18:BN:22:SER:OG	18:BN:25:ASN:N	2.46	0.45
5:AA:435:A:O2'	5:AA:436:A:OP1	2.24	0.45
5:AA:542:G:N1	5:AA:605:C:N3	2.64	0.45
5:AA:984:C:O2'	28:AX:30:PHE:O	2.34	0.45
10:AF:185:VAL:HG11	10:AF:230:ALA:HB1	1.98	0.45
11:AG:51:ASP:OD1	11:AG:51:ASP:N	2.45	0.45
5:BA:557:G:N1	5:BA:589:U:N3	2.65	0.45
13:BI:111:ILE:HD11	13:BI:122:VAL:HB	1.98	0.45
3:A4:133:LEU:HD21	3:A4:209:LEU:HD21	1.99	0.45
5:AA:557:G:C2	5:AA:589:U:C2	3.05	0.45
5:AA:705:C:OP1	22:AR:79:THR:OG1	2.32	0.45
5:AA:915:U:H1'	25:AU:113:VAL:HG13	1.99	0.45
5:AA:1334:A:H2	13:AI:73:ARG:HE	1.64	0.45
5:BA:693:C:O2'	22:BR:108:HIS:ND1	2.35	0.45
16:BL:17:ALA:CB	16:BL:64:VAL:HG12	2.46	0.45
24:BT:17:VAL:HG21	24:BT:57:LEU:HD22	1.98	0.45
30:BZ:41:ILE:HD12	30:BZ:63:GLU:HG2	1.97	0.45
5:AA:433:U:H3'	5:AA:434:A:H4'	1.98	0.45
5:AA:534:G:HO2'	5:AA:535:U:C5'	2.29	0.45
5:AA:584:C:HO2'	5:AA:585:U:H5	1.61	0.45
5:AA:937:A:H61	5:AA:1276:G:H1'	1.81	0.45
7:AC:122:ASN:OD1	7:AC:122:ASN:N	2.49	0.45
9:AE:36:LYS:N	9:AE:40:GLU:OE2	2.49	0.45
15:AK:40:GLN:OE1	15:AK:40:GLN:N	2.49	0.45
5:BA:5:C:O2	5:BA:459:G:O2'	2.35	0.45
5:BA:323:A:O2'	5:BA:324:C:O4'	2.32	0.45
5:BA:410:U:H2'	5:BA:413:G:H21	1.82	0.45
5:BA:689:C:O3'	8:BD:138:ARG:NH1	2.49	0.45
5:BA:866:A:OP1	19:BO:31:LYS:NZ	2.42	0.45
5:BA:983:G:O2'	5:BA:984:C:O4'	2.27	0.45
6:BB:60:ALA:HB2	6:BB:175:ILE:HA	1.98	0.45
12:BH:41:LYS:HA	12:BH:41:LYS:HE3	1.97	0.45
13:BI:18:MET:SD	13:BI:19:GLY:N	2.89	0.45
5:AA:614:G:H21	29:AY:49:GLY:HA2	1.81	0.45
5:AA:656:U:O4	3:B4:27:ARG:NH2	2.49	0.45
5:AA:1339:G:O2'	30:AZ:21:THR:O	2.25	0.45
27:AW:33:ARG:NH1	27:AW:53:ILE:O	2.50	0.45
3:B3:186:ILE:HD13	3:B3:200:GLY:HA3	1.99	0.45
5:BA:404:C:OP1	9:BE:117:THR:OG1	2.25	0.45
5:BA:605:C:OP1	22:BR:75:ASN:ND2	2.38	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BA:768:A:N6	5:BA:770:A:N3	2.64	0.45
11:BG:86:LEU:HD11	11:BG:98:LEU:HD11	1.99	0.45
23:BS:46:THR:HG23	23:BS:98:LYS:HE2	1.99	0.45
4:A5:60:GLU:O	4:A5:64:ALA:N	2.49	0.45
5:AA:963:A:H2'	5:AA:987:G:H22	1.81	0.45
5:AA:967:C:HO2'	5:AA:968:C:C1'	2.27	0.45
20:AP:80:ASN:OD1	20:AP:81:ARG:N	2.50	0.45
3:B4:182:SER:OG	3:B4:201:LEU:HD12	2.16	0.45
20:BP:14:ASP:O	20:BP:15:LEU:HD23	2.17	0.45
26:BV:10:ASP:O	26:BV:13:VAL:HG12	2.16	0.45
3:A3:186:ILE:HD13	3:A3:200:GLY:N	2.31	0.45
5:AA:1276:G:N7	25:AU:38:ARG:NH1	2.64	0.45
10:AF:127:ILE:HD12	10:AF:162:TYR:HB2	1.98	0.45
12:AH:88:LEU:HD22	12:AH:94:PHE:HB2	1.98	0.45
13:AI:9:PHE:CZ	16:AL:46:LEU:HD13	2.52	0.45
14:AJ:24:GLU:OE1	14:AJ:64:GLN:NE2	2.49	0.45
5:BA:821:G:N2	5:BA:824:G:OP2	2.44	0.45
5:BA:1392:G:O2'	5:BA:1423:A:N6	2.44	0.45
9:AE:59:LEU:O	9:AE:62:ARG:NH2	2.42	0.45
9:AE:104:ARG:NH2	9:AE:140:PRO:O	2.50	0.45
14:AJ:18:GLU:O	14:AJ:21:GLY:N	2.50	0.45
14:AJ:75:ILE:HD12	14:AJ:93:PHE:CZ	2.52	0.45
3:B4:37:THR:O	3:B4:40:THR:OG1	2.32	0.45
5:BA:1060:G:OP1	7:BC:153:LYS:N	2.49	0.45
9:BE:96:THR:OG1	9:BE:99:ASP:OD1	2.19	0.45
14:BJ:3:LEU:HD12	14:BJ:4:LEU:N	2.31	0.45
15:BK:35:THR:HG22	15:BK:57:LEU:O	2.17	0.45
22:BR:105:LEU:HD11	22:BR:109:LEU:HD21	1.99	0.45
3:A3:36:ASP:O	3:A3:40:THR:OG1	2.30	0.45
5:AA:839:G:H2'	5:AA:840:C:O4'	2.17	0.45
5:AA:1182:G:OP1	5:AA:1281:U:O2'	2.32	0.45
15:AK:3:ILE:O	15:AK:29:GLY:N	2.40	0.45
30:AZ:18:THR:OG1	30:AZ:19:GLY:N	2.51	0.45
4:B5:115:ALA:O	4:B5:119:LYS:N	2.46	0.45
5:BA:1310:C:HO2'	13:BI:94:ASN:CG	2.13	0.45
5:BA:1480:G:N7	18:BN:132:ARG:NH1	2.66	0.45
3:A3:238:ILE:HD11	3:A3:279:VAL:CG2	2.48	0.44
5:AA:232:G:C5'	23:AS:70:ILE:HD11	2.47	0.44
5:AA:249:U:O4'	5:AA:271:G:N2	2.45	0.44
5:AA:358:G:N2	5:AA:361:A:OP2	2.44	0.44
5:AA:613:C:O2	29:AY:32:ALA:HB1	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AA:1007:A:N3	7:AC:135:LYS:NZ	2.50	0.44
13:AI:129:ASN:ND2	13:AI:192:ALA:O	2.50	0.44
14:AJ:3:LEU:HD12	14:AJ:4:LEU:N	2.32	0.44
27:AW:3:ILE:HD11	27:AW:36:VAL:HG23	1.99	0.44
3:B3:35:VAL:HG11	3:B3:125:LEU:HD21	1.98	0.44
5:BA:400:G:H1	5:BA:451:A:H62	1.65	0.44
4:A5:114:ILE:O	4:A5:118:VAL:N	2.50	0.44
5:AA:869:U:OP2	19:AO:123:ARG:NH2	2.50	0.44
5:AA:898:G:O2'	5:AA:1335:A:N3	2.45	0.44
5:AA:1307:G:O2'	5:AA:1308:U:OP2	2.35	0.44
11:AG:61:GLU:OE1	11:AG:61:GLU:N	2.50	0.44
3:B3:179:MET:SD	3:B3:183:ILE:HD11	2.57	0.44
4:B5:78:ILE:HD12	4:B5:114:ILE:HG23	2.00	0.44
5:BA:615:G:O6	5:BA:698:A:C6	2.69	0.44
6:BB:62:PHE:HB2	6:BB:67:ILE:HD11	1.98	0.44
17:BM:19:VAL:HG21	17:BM:96:ILE:HD11	1.99	0.44
5:AA:1260:G:O2'	5:AA:1261:U:OP2	2.27	0.44
8:AD:108:ASN:OD1	8:AD:108:ASN:N	2.50	0.44
11:AG:88:ALA:HB2	11:AG:98:LEU:HD13	1.99	0.44
5:BA:462:A:O4'	5:BA:496:C:O2'	2.34	0.44
5:BA:703:U:OP1	22:BR:16:ARG:NH2	2.50	0.44
6:BB:86:VAL:HG11	6:BB:172:ALA:HB1	1.99	0.44
20:BP:5:ARG:N	20:BP:52:GLY:O	2.51	0.44
5:AA:1018:C:N4	5:AA:1151:A:C6	2.85	0.44
5:BA:442:C:O2'	27:BW:28:GLU:O	2.34	0.44
5:BA:962:G:N3	5:BA:988:A:N6	2.66	0.44
10:BF:46:LEU:HA	10:BF:49:VAL:HG12	1.99	0.44
22:BR:96:MET:HA	22:BR:99:ILE:HD12	1.99	0.44
3:A3:182:SER:O	3:A3:186:ILE:HG22	2.17	0.44
5:AA:421:U:H3	5:AA:448:A:H62	1.64	0.44
5:AA:966:G:H21	28:AX:41:GLY:C	2.21	0.44
25:AU:72:ILE:HG21	25:AU:98:MET:HB3	2.00	0.44
27:AW:5:ILE:HD12	27:AW:19:ILE:HD11	1.99	0.44
5:BA:310:G:N7	10:BF:2:ALA:N	2.65	0.44
5:BA:516:A:O4'	5:BA:519:G:N2	2.50	0.44
11:BG:213:ILE:HD13	11:BG:223:ILE:HD13	1.99	0.44
26:BV:58:ILE:HD11	26:BV:73:LEU:HD13	1.99	0.44
29:BY:63:GLU:N	29:BY:63:GLU:OE2	2.50	0.44
5:AA:232:G:H5"	23:AS:70:ILE:HD11	1.98	0.44
5:AA:331:C:OP1	12:AH:85:ARG:NH2	2.49	0.44
22:AR:136:TYR:O	22:AR:140:GLY:N	2.43	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:AX:33:ASP:OD1	28:AX:33:ASP:N	2.41	0.44
29:AY:37:CYS:HB2	29:AY:44:LEU:HD21	1.98	0.44
5:BA:699:C:N4	5:BA:700:G:O6	2.51	0.44
7:BC:195:ILE:HD11	24:BT:16:LEU:HD12	2.00	0.44
9:BE:70:ARG:HG3	9:BE:89:LEU:HD13	1.99	0.44
13:BI:71:ILE:HD11	13:BI:180:PHE:HE2	1.82	0.44
5:AA:539:C:O2'	5:AA:836:G:H4'	2.18	0.44
8:AD:17:GLN:OE1	8:AD:17:GLN:N	2.50	0.44
23:AS:41:ASP:OD1	23:AS:41:ASP:N	2.46	0.44
27:AW:38:GLY:O	27:AW:41:VAL:HG12	2.18	0.44
3:B3:133:LEU:HD11	3:B3:143:TYR:HB2	1.99	0.44
4:B5:68:PRO:HG2	28:BX:10:ILE:HD13	2.00	0.44
4:B5:94:VAL:HG21	5:BA:960:A:O2'	2.18	0.44
5:BA:894:A:H2'	5:BA:895:C:O4'	2.18	0.44
5:BA:1327:C:OP1	16:BL:120:ASN:N	2.51	0.44
18:BN:107:ARG:O	30:BZ:35:ARG:NH1	2.46	0.44
3:A3:89:PHE:CD2	3:A3:139:ALA:HB2	2.52	0.44
3:A4:222:LYS:O	3:A4:223:LEU:HD22	2.18	0.44
4:A5:52:ILE:HD12	4:A5:99:VAL:O	2.18	0.44
5:AA:1460:G:HO2'	5:AA:1461:U:P	2.29	0.44
13:AI:209:ARG:O	13:AI:211:ALA:N	2.49	0.44
17:AM:12:ASN:ND2	17:AM:15:SER:OG	2.51	0.44
1:B1:11:CYS:SG	1:B1:13:SER:OG	2.66	0.44
3:B3:180:LEU:HA	3:B3:183:ILE:HD12	1.99	0.44
5:BA:1421:C:O4'	15:BK:2:ALA:N	2.51	0.44
10:BF:185:VAL:CG2	10:BF:199:ILE:HD11	2.47	0.44
18:BN:25:ASN:OD1	18:BN:26:THR:N	2.48	0.44
5:AA:1228:A:OP1	26:AV:96:SER:N	2.46	0.44
1:B1:46:LEU:O	1:B1:46:LEU:HD23	2.18	0.44
5:BA:1206:G:H4'	26:BV:13:VAL:HG11	2.00	0.44
20:BP:107:MET:SD	20:BP:111:ARG:NH2	2.91	0.44
3:A3:135:VAL:HG12	3:A3:136:ASP:H	1.83	0.43
3:A3:140:ARG:NH2	3:A3:245:GLY:O	2.51	0.43
5:AA:250:G:O2'	23:AS:44:ARG:O	2.34	0.43
5:AA:583:G:O6	5:AA:584:C:N4	2.51	0.43
5:AA:1205:G:H21	26:AV:10:ASP:CG	2.21	0.43
26:AV:106:GLU:OE1	26:AV:119:ARG:NE	2.44	0.43
3:B3:96:ILE:O	3:B3:96:ILE:HG13	2.18	0.43
5:BA:998:A:H62	5:BA:1171:G:H21	1.66	0.43
5:BA:1227:A:H61	5:BA:1287:G:H1'	1.83	0.43
5:BA:1334:A:N3	13:BI:73:ARG:NE	2.66	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:BJ:66:LEU:HB2	14:BJ:68:ARG:HE	1.83	0.43
24:BT:8:PHE:CZ	24:BT:9:ILE:HD11	2.53	0.43
5:AA:454:G:OP1	19:AO:135:LYS:NZ	2.46	0.43
9:AE:130:ILE:HD11	9:AE:152:ILE:HG22	1.99	0.43
3:B3:188:GLU:O	3:B3:192:TYR:N	2.52	0.43
5:BA:932:C:H3'	5:BA:933:G:H5"	2.00	0.43
24:BT:29:GLU:OE1	24:BT:29:GLU:N	2.50	0.43
13:AI:107:ALA:HA	13:AI:110:ILE:HD12	1.98	0.43
3:B4:130:LEU:HD11	3:B4:278:LEU:CD2	2.49	0.43
5:BA:513:A:N6	5:BA:519:G:OP1	2.51	0.43
5:BA:1016:G:O3'	5:BA:1150:G:N2	2.52	0.43
3:A4:4:VAL:HG22	3:A4:4:VAL:O	2.18	0.43
5:AA:891:A:O2'	5:AA:894:A:N6	2.46	0.43
6:AB:51:ARG:NH1	6:AB:153:ALA:O	2.51	0.43
7:AC:34:ASP:OD1	7:AC:35:ILE:N	2.51	0.43
7:AC:168:GLN:NE2	7:AC:175:VAL:HG11	2.34	0.43
29:AY:48:THR:CG2	29:AY:53:ILE:HD11	2.49	0.43
5:BA:3:U:O4	9:BE:22:ARG:NH2	2.52	0.43
5:BA:111:G:HO2'	5:BA:112:G:P	2.39	0.43
9:BE:90:ASP:O	11:BG:161:ARG:NH2	2.47	0.43
5:AA:1211:A:N3	5:AA:1329:C:O2'	2.36	0.43
6:AB:28:MET:N	6:AB:28:MET:SD	2.92	0.43
15:AK:41:ASP:OD1	15:AK:61:ALA:N	2.47	0.43
22:AR:129:ILE:HD12	22:AR:148:TYR:CZ	2.53	0.43
5:BA:517:U:O2'	23:BS:62:ARG:NH2	2.52	0.43
5:AA:140:C:N4	5:AA:152:G:O6	2.50	0.43
5:AA:655:A:HO2'	5:AA:656:U:P	2.33	0.43
5:AA:672:G:HO2'	5:AA:673:C:P	2.36	0.43
5:AA:985:C:O3'	5:AA:986:G:N2	2.51	0.43
10:AF:106:ARG:NH1	10:AF:194:ALA:O	2.52	0.43
21:AQ:36:LEU:HD12	21:AQ:36:LEU:H	1.84	0.43
10:BF:55:TYR:O	27:BW:11:ASN:ND2	2.52	0.43
2:A2:26:LEU:HD21	2:A2:30:ARG:HH21	1.84	0.43
3:A3:251:SER:OG	3:A3:252:ILE:N	2.52	0.43
6:AB:68:LEU:HD21	6:AB:110:PHE:HD2	1.82	0.43
25:AU:13:LEU:HA	25:AU:16:LEU:HD12	1.99	0.43
6:BB:182:ILE:HG23	6:BB:187:ASP:OD1	2.18	0.43
3:A3:255:GLU:O	3:A3:259:ASN:ND2	2.51	0.43
5:BA:998:A:H62	5:BA:1171:G:N2	2.17	0.43
13:BI:47:THR:HG23	13:BI:49:GLY:N	2.32	0.43
17:BM:5:ARG:HG3	17:BM:72:LEU:HD11	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A2:28:ARG:HE	5:AA:860:G:P	2.41	0.43
14:AJ:28:LYS:NZ	14:AJ:58:ALA:HB3	2.32	0.43
17:AM:93:ASP:OD1	17:AM:94:VAL:HG23	2.19	0.43
21:AQ:39:CYS:SG	21:AQ:42:CYS:N	2.77	0.43
25:AU:66:HIS:O	25:AU:68:ARG:N	2.50	0.43
2:B2:1:MET:HB2	5:BA:861:G:OP1	2.19	0.43
3:B3:64:ASN:ND2	5:BA:763:G:OP1	2.52	0.43
5:BA:252:U:OP2	23:BS:20:LYS:NZ	2.52	0.43
5:BA:458:G:H3'	5:BA:459:G:H21	1.83	0.43
5:BA:606:U:O2'	5:BA:607:U:O2	2.25	0.43
21:BQ:24:CYS:SG	21:BQ:25:GLY:N	2.92	0.43
5:AA:655:A:N3	3:B4:218:ARG:NH2	2.67	0.43
11:AG:131:TRP:NE1	14:AJ:90:GLU:OE2	2.41	0.43
18:AN:135:ARG:O	18:AN:137:VAL:N	2.49	0.43
3:B4:142:VAL:HG11	3:B4:205:ALA:HB1	2.00	0.43
3:B4:233:ARG:NH1	3:B4:263:THR:OG1	2.51	0.43
4:B5:43:VAL:HG13	4:B5:75:ILE:HD12	1.99	0.43
6:BB:138:VAL:HG22	6:BB:152:LEU:HB3	2.01	0.43
9:BE:80:LEU:HB2	9:BE:82:LEU:HD23	2.01	0.43
9:BE:82:LEU:CB	9:BE:83:LEU:HD22	2.49	0.43
10:BF:166:MET:SD	10:BF:167:LYS:N	2.92	0.43
22:BR:70:ASP:OD2	22:BR:84:LYS:NZ	2.36	0.43
26:BV:74:ARG:HG3	26:BV:98:ILE:HD11	2.01	0.43
3:A3:161:LEU:O	3:A3:165:SER:OG	2.37	0.42
5:AA:661:C:O2'	18:AN:35:GLY:O	2.28	0.42
5:AA:1053:A:O2'	5:AA:1054:A:OP2	2.23	0.42
26:AV:47:GLN:OE1	26:AV:47:GLN:N	2.45	0.42
5:BA:29:G:O6	5:BA:502:U:C4	2.72	0.42
5:BA:89:G:N2	5:BA:375:G:O2'	2.52	0.42
5:BA:123:U:O2'	10:BF:171:ARG:NH1	2.52	0.42
5:BA:152:G:C6	5:BA:153:G:O6	2.71	0.42
5:BA:1271:G:OP1	25:BU:9:ARG:NH2	2.52	0.42
10:BF:53:LEU:HD13	10:BF:55:TYR:CE2	2.54	0.42
13:BI:32:SER:HA	30:BZ:54:ILE:HB	2.01	0.42
3:A4:281:VAL:O	3:A4:285:ASN:ND2	2.44	0.42
5:AA:194:C:O2'	15:AK:43:ARG:NH1	2.52	0.42
5:AA:251:G:OP1	23:AS:98:LYS:NZ	2.33	0.42
5:AA:1121:C:OP1	24:AT:59:ARG:NH2	2.52	0.42
3:B3:136:ASP:O	3:B3:293:LEU:HD23	2.19	0.42
5:BA:85:A:H2'	5:BA:86:C:C6	2.54	0.42
5:BA:702:G:N2	5:BA:706:G:O6	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BA:1251:C:H2'	5:BA:1252:C:O4'	2.19	0.42
10:BF:39:MET:SD	10:BF:40:ARG:N	2.93	0.42
19:BO:30:TYR:CE1	19:BO:34:VAL:HG11	2.55	0.42
3:A3:28:LEU:O	3:A3:28:LEU:HD23	2.20	0.42
3:A4:135:VAL:HG21	3:A4:289:ILE:HD12	2.01	0.42
3:A4:186:ILE:HD13	3:A4:202:VAL:HG12	2.01	0.42
4:A5:50:LEU:HD13	4:A5:111:VAL:HG13	2.01	0.42
27:AW:78:MET:HE3	27:AW:92:LEU:HD13	2.01	0.42
1:B1:21:ARG:HG3	11:BG:122:ILE:HG22	2.01	0.42
5:BA:985:C:H2'	5:BA:986:G:C2	2.54	0.42
5:BA:1246:U:HO2'	26:BV:90:PHE:HZ	1.67	0.42
5:BA:1289:G:H1'	20:BP:98:LEU:HD21	2.00	0.42
19:BO:34:VAL:HG23	19:BO:35:LEU:HD22	2.00	0.42
19:BO:57:LYS:HD3	19:BO:94:ILE:HD11	2.02	0.42
1:A1:46:LEU:HD13	1:A1:48:LYS:HZ2	1.84	0.42
5:AA:720:A:N7	5:AA:767:U:O4	2.53	0.42
5:AA:973:U:N3	5:AA:975:A:O5'	2.52	0.42
5:AA:1378:A:H61	5:AA:1437:G:C2'	2.32	0.42
9:AE:161:ALA:O	9:AE:168:ARG:NH1	2.52	0.42
10:AF:202:ILE:HD12	10:AF:213:VAL:HG12	2.02	0.42
3:B3:161:LEU:O	3:B3:165:SER:OG	2.26	0.42
5:BA:376:G:N2	5:BA:379:A:OP2	2.52	0.42
5:BA:548:A:N3	5:BA:549:A:N6	2.65	0.42
5:BA:951:G:N2	5:BA:1171:G:H2'	2.34	0.42
5:BA:1165:U:O4'	7:BC:175:VAL:HG21	2.19	0.42
5:BA:1470:G:N2	5:BA:1471:G:C2	2.87	0.42
16:BL:64:VAL:HG11	16:BL:82:ILE:CD1	2.49	0.42
18:BN:29:HIS:CE1	18:BN:38:THR:HG1	2.37	0.42
20:BP:43:ALA:HB1	20:BP:61:LYS:CE	2.49	0.42
22:BR:37:VAL:HG11	22:BR:81:ILE:HG21	2.00	0.42
3:A3:268:THR:HG21	3:A3:272:GLU:OE1	2.19	0.42
5:AA:324:C:O2'	5:AA:325:A:OP2	2.29	0.42
5:AA:526:A:H2'	5:AA:527:A:O4'	2.19	0.42
5:AA:699:C:OP2	22:AR:12:SER:N	2.52	0.42
5:AA:999:G:N2	5:AA:1173:A:N1	2.67	0.42
8:AD:120:MET:SD	8:AD:187:LYS:HB3	2.59	0.42
12:AH:63:ILE:HA	12:AH:121:VAL:HG12	2.01	0.42
5:BA:1097:G:H21	26:BV:3:THR:CG2	2.32	0.42
7:BC:99:LEU:HD23	7:BC:178:VAL:HG21	2.02	0.42
3:A3:125:LEU:HD12	3:A3:129:LEU:HD13	2.01	0.42
5:AA:1198:A:H5"	5:AA:1259:A:H61	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AA:1486:A:H2'	5:AA:1487:U:C6	2.55	0.42
19:AO:136:GLU:OE1	19:AO:136:GLU:N	2.48	0.42
22:AR:29:THR:OG1	22:AR:30:VAL:N	2.51	0.42
29:AY:43:THR:HG23	29:AY:55:LYS:HD3	2.01	0.42
5:BA:166:A:H61	5:BA:196:G:C2'	2.32	0.42
5:BA:247:G:N1	5:BA:262:G:O6	2.53	0.42
5:BA:1170:C:HO2'	5:BA:1173:A:HO2'	1.66	0.42
7:BC:21:LEU:HD13	7:BC:46:ILE:HD12	2.01	0.42
11:BG:164:GLY:N	11:BG:182:ASP:OD1	2.52	0.42
13:BI:72:MET:O	13:BI:94:ASN:ND2	2.53	0.42
20:BP:22:ARG:O	20:BP:26:THR:HG23	2.20	0.42
5:AA:984:C:O3'	28:AX:30:PHE:HB2	2.20	0.42
5:AA:1296:U:OP2	13:AI:175:ARG:NE	2.52	0.42
18:AN:124:ASP:OD1	18:AN:124:ASP:N	2.53	0.42
20:AP:114:ALA:O	20:AP:117:GLY:N	2.53	0.42
24:AT:8:PHE:O	24:AT:12:VAL:HG12	2.19	0.42
5:BA:234:G:OP1	23:BS:66:ARG:NH1	2.47	0.42
5:BA:1357:C:OP2	11:BG:79:ARG:NH2	2.53	0.42
8:BD:141:MET:HE2	8:BD:170:ILE:HD12	2.02	0.42
9:BE:10:LYS:O	9:BE:46:THR:HG21	2.19	0.42
5:AA:1260:G:N1	5:AA:1295:C:O4'	2.51	0.42
5:AA:1335:A:N3	13:AI:73:ARG:NH2	2.67	0.42
5:AA:1414:G:OP1	12:AH:86:VAL:HG13	2.19	0.42
10:AF:46:LEU:HD11	10:AF:50:ARG:HD2	2.01	0.42
16:AL:118:LYS:HD2	16:AL:119:PRO:O	2.20	0.42
30:AZ:12:ILE:HD11	30:AZ:30:ARG:HB2	2.01	0.42
5:BA:480:G:O2'	5:BA:488:A:N1	2.42	0.42
5:BA:905:A:O2'	5:BA:1293:A:N3	2.44	0.42
8:BD:46:ARG:NH1	18:BN:37:GLU:OE2	2.53	0.42
13:BI:45:PRO:CB	13:BI:64:VAL:HG23	2.48	0.42
14:BJ:4:LEU:N	14:BJ:4:LEU:HD22	2.35	0.42
5:AA:778:G:OP1	22:AR:3:ARG:NE	2.52	0.42
8:AD:112:LYS:NZ	8:AD:151:GLU:O	2.28	0.42
27:AW:77:ARG:NH1	27:AW:81:ILE:HD11	2.35	0.42
30:AZ:23:ASP:N	30:AZ:23:ASP:OD1	2.52	0.42
2:B2:21:LYS:NZ	5:BA:1470:G:O6	2.52	0.42
3:B4:214:LEU:HD21	3:B4:225:VAL:HG13	2.01	0.42
4:B5:32:ILE:HG22	4:B5:101:ILE:HG12	2.01	0.42
5:BA:297:G:H5"	23:BS:59:LYS:HZ3	1.85	0.42
13:BI:146:TYR:OH	30:BZ:65:ARG:NH1	2.52	0.42
18:BN:91:SER:OG	18:BN:92:LYS:N	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BU:93:GLU:OE2	25:BU:94:ILE:N	2.53	0.42
2:A2:26:LEU:HD11	2:A2:30:ARG:HH21	1.84	0.42
5:AA:73:U:O2	5:AA:77:G:C2	2.73	0.42
8:AD:51:THR:OG1	8:AD:54:ASP:OD2	2.28	0.42
23:AS:21:CYS:O	23:AS:25:GLY:N	2.53	0.42
5:BA:707:A:OP1	22:BR:139:LYS:NZ	2.46	0.42
10:BF:74:ASP:OD2	10:BF:123:LYS:NZ	2.34	0.42
10:BF:164:VAL:HG13	10:BF:173:ILE:HG23	2.00	0.42
19:BO:76:GLN:NE2	19:BO:77:LEU:O	2.48	0.42
29:BY:59:LEU:H	29:BY:59:LEU:HD12	1.85	0.42
1:A1:46:LEU:H	1:A1:46:LEU:HD12	1.83	0.41
3:A3:201:LEU:HA	3:A3:204:VAL:HG12	2.01	0.41
5:AA:372:G:OP1	10:AF:47:TYR:OH	2.27	0.41
5:AA:719:G:P	22:AR:116:LEU:HD13	2.60	0.41
10:AF:167:LYS:O	10:AF:171:ARG:N	2.52	0.41
12:AH:38:ILE:HD12	12:AH:39:PRO:HD2	2.01	0.41
3:B4:4:VAL:CG2	3:B4:201:LEU:HD11	2.50	0.41
5:BA:1481:G:N7	18:BN:132:ARG:NH2	2.60	0.41
14:BJ:111:MET:SD	14:BJ:111:MET:N	2.93	0.41
3:A4:57:ASN:OD1	3:A4:57:ASN:N	2.52	0.41
5:AA:561:A:O2'	10:AF:13:LEU:O	2.34	0.41
12:AH:67:THR:HG22	12:AH:73:PRO:HD3	2.01	0.41
3:B3:233:ARG:NH2	3:B3:260:LEU:O	2.53	0.41
3:B4:293:LEU:HA	3:B4:296:MET:HB2	2.01	0.41
5:BA:917:A:H62	25:BU:111:LYS:CE	2.32	0.41
10:BF:168:VAL:N	10:BF:169:PRO:HD2	2.36	0.41
24:BT:9:ILE:HD13	24:BT:9:ILE:N	2.35	0.41
5:AA:257:U:OP2	15:AK:116:GLN:NE2	2.49	0.41
5:AA:640:U:O4	5:AA:657:A:O2'	2.19	0.41
7:AC:17:ILE:HD11	7:AC:75:LEU:HD11	2.01	0.41
27:AW:21:PHE:HE2	27:AW:23:ILE:HD11	1.86	0.41
29:AY:33:THR:OG1	29:AY:34:LYS:N	2.53	0.41
3:B4:157:LYS:HA	3:B4:160:ILE:HG22	2.02	0.41
5:BA:535:U:H3	5:BA:713:A:H62	1.66	0.41
3:A3:237:GLU:OE1	3:A3:238:ILE:N	2.53	0.41
3:A4:119:LEU:H	3:A4:119:LEU:HD12	1.85	0.41
5:AA:288:G:OP2	5:AA:301:G:N1	2.44	0.41
23:AS:51:ARG:NE	23:AS:51:ARG:HA	2.35	0.41
27:AW:11:ASN:OD1	27:AW:16:ARG:NH2	2.53	0.41
3:B4:6:ILE:HB	3:B4:199:ILE:HG22	2.02	0.41
5:BA:368:C:N4	5:BA:384:G:OP2	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:BA:609:G:OP1	22:BR:3:ARG:NH1	2.53	0.41
5:BA:671:C:HO2'	5:BA:688:C:H6	1.68	0.41
5:BA:1026:A:H61	5:BA:1035:C:N4	2.18	0.41
5:BA:1197:C:HO2'	5:BA:1260:G:H22	1.60	0.41
11:BG:43:GLN:OE1	11:BG:43:GLN:N	2.53	0.41
14:BJ:37:VAL:HG23	14:BJ:103:ILE:HD13	2.02	0.41
3:A4:277:LEU:O	3:A4:277:LEU:HD23	2.20	0.41
5:AA:882:C:O2'	5:AA:1457:A:N7	2.50	0.41
5:AA:1305:U:HO2'	5:AA:1337:A:H2	1.66	0.41
8:AD:122:MET:SD	8:AD:123:ALA:N	2.94	0.41
3:B4:232:LEU:HD22	3:B4:260:LEU:HD21	2.02	0.41
5:BA:453:G:H2'	5:BA:454:G:O4'	2.20	0.41
5:BA:1053:A:O2'	5:BA:1054:A:OP2	2.30	0.41
11:BG:20:THR:OG1	11:BG:21:LYS:N	2.53	0.41
22:BR:95:LEU:HD23	22:BR:99:ILE:CD1	2.51	0.41
5:AA:288:G:O2'	5:AA:561:A:N6	2.50	0.41
5:AA:421:U:O4	5:AA:448:A:N7	2.53	0.41
5:AA:1126:G:N2	5:AA:1129:A:OP2	2.48	0.41
6:AB:69:ALA:HB1	6:AB:80:VAL:HG23	2.02	0.41
11:AG:136:ARG:NE	11:AG:219:GLU:O	2.49	0.41
5:BA:342:G:N2	5:BA:343:G:N7	2.68	0.41
6:AB:111:GLU:OE2	11:AG:20:THR:OG1	2.33	0.41
1:B1:22:GLU:HG3	1:B1:41:GLU:HB2	2.03	0.41
4:B5:47:GLN:HB3	4:B5:102:ILE:HG23	2.02	0.41
6:BB:163:ALA:O	6:BB:167:ILE:HG12	2.21	0.41
4:A5:6:TYR:HD2	4:A5:67:PRO:HG2	1.86	0.41
5:AA:939:C:HO2'	5:AA:940:U:P	2.38	0.41
23:AS:85:LYS:O	23:AS:106:LEU:N	2.54	0.41
28:AX:31:MET:HB3	28:AX:38:TRP:CE3	2.56	0.41
5:BA:530:G:H22	5:BA:718:G:H22	1.68	0.41
5:BA:1167:C:OP1	7:BC:172:LYS:NZ	2.33	0.41
7:BC:14:GLU:CG	7:BC:35:ILE:HD12	2.49	0.41
13:BI:209:ARG:O	13:BI:211:ALA:N	2.53	0.41
17:BM:40:LEU:HD22	17:BM:70:LYS:HB3	2.01	0.41
3:A3:222:LYS:O	3:A3:223:LEU:HD22	2.21	0.41
3:A4:284:GLU:N	3:A4:284:GLU:OE1	2.54	0.41
4:A5:112:GLU:O	4:A5:115:ALA:HB3	2.20	0.41
5:AA:43:A:HO2'	5:AA:44:C:P	2.44	0.41
5:AA:246:A:HO2'	5:AA:247:G:P	2.43	0.41
5:AA:246:A:O2'	5:AA:247:G:O5'	2.31	0.41
5:AA:422:U:H1'	5:AA:447:A:H62	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AA:540:G:N1	5:AA:708:C:OP2	2.43	0.41
5:AA:616:G:H22	5:AA:697:A:H2	1.69	0.41
5:AA:1006:C:O5'	5:AA:1156:A:O2'	2.39	0.41
5:AA:1170:C:O2'	5:AA:1173:A:N3	2.38	0.41
5:AA:1262:U:OP2	20:AP:19:LYS:NZ	2.41	0.41
8:AD:117:LEU:HD12	8:AD:189:LYS:O	2.21	0.41
12:AH:75:ARG:HB3	12:AH:78:ILE:HD12	2.03	0.41
13:AI:82:ALA:HB3	13:AI:84:HIS:HE1	1.86	0.41
19:AO:56:GLU:HG3	19:AO:74:ARG:HB2	2.03	0.41
20:AP:80:ASN:ND2	20:AP:93:LEU:O	2.54	0.41
22:AR:92:PRO:HG2	22:AR:136:TYR:CE1	2.56	0.41
22:AR:137:LYS:NZ	22:AR:142:LEU:O	2.53	0.41
23:AS:21:CYS:HG	23:AS:24:HIS:CG	2.33	0.41
23:AS:37:ILE:HD13	23:AS:85:LYS:HA	2.03	0.41
3:B3:289:ILE:HD13	3:B3:289:ILE:N	2.36	0.41
3:B4:186:ILE:HG21	3:B4:200:GLY:HA3	2.03	0.41
4:B5:48:ALA:HB3	4:B5:75:ILE:HD13	2.02	0.41
5:BA:89:G:H2'	5:BA:90:C:O4'	2.21	0.41
5:BA:150:G:N3	12:BH:120:ASN:ND2	2.59	0.41
5:BA:250:G:OP1	23:BS:97:THR:OG1	2.38	0.41
5:BA:298:C:P	23:BS:59:LYS:HZ1	2.42	0.41
5:BA:542:G:O6	5:BA:605:C:N4	2.54	0.41
5:BA:1226:G:O2'	5:BA:1228:A:N6	2.46	0.41
5:BA:1373:A:H2'	5:BA:1374:C:O4'	2.21	0.41
17:BM:30:THR:O	17:BM:80:ARG:NH2	2.54	0.41
17:BM:87:ARG:HG3	17:BM:87:ARG:O	2.20	0.41
26:BV:25:GLU:HG3	26:BV:108:ALA:HB2	2.03	0.41
26:BV:106:GLU:OE1	26:BV:119:ARG:NH2	2.51	0.41
3:A4:134:LEU:HD13	3:A4:282:ILE:HG13	2.03	0.41
5:AA:1206:G:H4'	26:AV:13:VAL:HG21	2.03	0.41
5:AA:1210:A:H2'	5:AA:1211:A:C8	2.56	0.41
24:AT:62:MET:SD	24:AT:62:MET:N	2.90	0.41
29:AY:18:CYS:SG	29:AY:19:ILE:N	2.94	0.41
3:B3:51:ILE:HD11	3:B4:185:PHE:O	2.21	0.41
5:BA:1226:G:C2'	5:BA:1228:A:H62	2.34	0.41
14:BJ:38:LEU:HD13	14:BJ:61:TYR:CD2	2.56	0.41
20:BP:80:ASN:OD1	20:BP:93:LEU:HD12	2.21	0.41
27:BW:82:GLU:HB3	27:BW:86:ILE:HD11	2.03	0.41
5:AA:128:A:H2	5:AA:216:G:H22	1.70	0.40
9:AE:116:ARG:NE	9:AE:174:ALA:HB2	2.36	0.40
26:AV:58:ILE:O	26:AV:62:VAL:HG23	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B3:69:VAL:HG22	3:B3:69:VAL:O	2.21	0.40
10:BF:181:LYS:NZ	10:BF:201:GLU:OE1	2.54	0.40
20:BP:14:ASP:OD1	20:BP:15:LEU:N	2.54	0.40
20:BP:109:LEU:HD23	20:BP:112:ILE:HD11	2.02	0.40
5:AA:908:G:HO2'	5:AA:930:G:H1	1.68	0.40
5:AA:965:G:N2	5:AA:986:G:N7	2.68	0.40
5:AA:1060:G:OP1	7:AC:153:LYS:N	2.51	0.40
5:AA:1346:C:H2'	5:AA:1347:U:C6	2.56	0.40
13:AI:9:PHE:HE1	16:AL:46:LEU:HD13	1.84	0.40
14:AJ:86:PHE:HD2	14:AJ:117:ILE:HD11	1.86	0.40
1:B1:50:TYR:OH	6:BB:151:ASP:OD1	2.39	0.40
3:B3:184:LYS:HD3	3:B4:299:ILE:HD13	2.03	0.40
5:BA:32:A:H2'	5:BA:33:U:O4'	2.21	0.40
5:BA:166:A:N3	5:BA:197:A:N6	2.69	0.40
5:BA:1260:G:N2	5:BA:1295:C:O4'	2.54	0.40
20:BP:93:LEU:HB2	20:BP:98:LEU:HG	2.03	0.40
22:BR:19:ARG:NE	22:BR:21:ALA:O	2.55	0.40
24:BT:36:GLN:OE1	24:BT:37:GLU:N	2.54	0.40
26:BV:55:VAL:HG13	26:BV:105:LEU:HD11	2.02	0.40
27:BW:87:LEU:HB2	27:BW:93:ILE:HD12	2.03	0.40
3:A3:235:LEU:HA	3:A3:238:ILE:HG22	2.04	0.40
5:AA:31:U:N3	5:AA:501:G:C6	2.89	0.40
5:AA:238:G:OP2	19:AO:21:LYS:NZ	2.52	0.40
5:AA:402:G:H21	9:AE:123:GLN:HE22	1.68	0.40
5:AA:531:G:O2'	5:AA:682:A:N3	2.43	0.40
5:AA:1131:G:H5'	24:AT:4:ILE:HD13	2.03	0.40
29:AY:19:ILE:H	29:AY:19:ILE:HD12	1.85	0.40
3:B4:273:GLU:O	3:B4:277:LEU:HG	2.21	0.40
5:BA:561:A:O2'	10:BF:13:LEU:O	2.36	0.40
5:BA:1194:C:H2'	5:BA:1195:U:O4'	2.21	0.40
8:BD:170:ILE:HD11	8:BD:183:ALA:HB1	2.03	0.40
9:BE:122:ARG:HA	9:BE:125:ILE:HD12	2.03	0.40
12:BH:68:ASP:OD1	12:BH:69:LYS:N	2.49	0.40
20:BP:43:ALA:HB1	20:BP:61:LYS:HD2	2.02	0.40
27:BW:52:VAL:HG11	27:BW:86:ILE:HD12	2.03	0.40
29:BY:23:ASN:OD1	29:BY:24:GLU:N	2.54	0.40
1:A1:28:ILE:HD12	1:A1:29:CYS:N	2.34	0.40
2:A2:11:LYS:O	2:A2:13:ARG:NH1	2.54	0.40
5:AA:31:U:N3	5:AA:32:A:N7	2.70	0.40
5:AA:32:A:N6	5:AA:501:G:O6	2.54	0.40
5:AA:130:G:N1	5:AA:163:C:N3	2.69	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AA:176:U:HO2'	5:AA:177:A:P	2.38	0.40
5:AA:180:G:H21	5:AA:182:A:H3'	1.86	0.40
5:AA:961:U:O2'	5:AA:962:G:OP1	2.28	0.40
5:AA:1173:A:O2'	5:AA:1174:A:O5'	2.35	0.40
6:AB:112:PRO:HG2	6:AB:135:ILE:HD13	2.04	0.40
7:AC:33:LEU:HD23	7:AC:35:ILE:HD11	2.03	0.40
11:AG:156:LEU:HD21	11:AG:167:ILE:HD12	2.02	0.40
1:B1:19:THR:HG23	1:B1:22:GLU:HB2	2.03	0.40
4:B5:27:ARG:NH1	4:B5:89:ALA:O	2.54	0.40
5:BA:1029:G:O2'	5:BA:1031:G:N7	2.54	0.40
9:BE:77:LEU:CD1	9:BE:83:LEU:HD23	2.49	0.40
28:BX:10:ILE:HD11	28:BX:15:VAL:HG12	2.03	0.40
30:BZ:20:THR:HG23	30:BZ:21:THR:CG2	2.52	0.40
5:AA:1214:G:N1	5:AA:1244:C:N3	2.70	0.40
5:AA:1307:G:O2'	5:AA:1308:U:P	2.79	0.40
5:AA:1421:C:H2'	5:AA:1422:G:O4'	2.22	0.40
14:AJ:71:LYS:NZ	14:AJ:130:TYR:OH	2.26	0.40
29:AY:58:ILE:HD11	29:AY:60:GLU:O	2.21	0.40
5:BA:1204:C:N4	5:BA:1205:G:O6	2.55	0.40
9:BE:135:GLN:NE2	27:BW:61:GLY:O	2.54	0.40
11:BG:118:LYS:HA	11:BG:121:ILE:HD11	2.04	0.40
17:BM:6:ILE:HG12	17:BM:98:ILE:HG23	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A1	58/60 (97%)	52 (90%)	6 (10%)	0	100	100
1	B1	58/60 (97%)	52 (90%)	6 (10%)	0	100	100
2	A2	33/37 (89%)	32 (97%)	1 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B2	33/37 (89%)	32 (97%)	1 (3%)	0	100	100
3	A3	294/306 (96%)	272 (92%)	22 (8%)	0	100	100
3	A4	287/306 (94%)	263 (92%)	22 (8%)	2 (1%)	19	54
3	B3	297/306 (97%)	273 (92%)	23 (8%)	1 (0%)	37	69
3	B4	285/306 (93%)	262 (92%)	23 (8%)	0	100	100
4	A5	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
4	B5	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
6	AB	195/202 (96%)	179 (92%)	16 (8%)	0	100	100
6	BB	195/202 (96%)	188 (96%)	7 (4%)	0	100	100
7	AC	193/210 (92%)	189 (98%)	4 (2%)	0	100	100
7	BC	193/210 (92%)	191 (99%)	2 (1%)	0	100	100
8	AD	182/198 (92%)	179 (98%)	3 (2%)	0	100	100
8	BD	182/198 (92%)	177 (97%)	5 (3%)	0	100	100
9	AE	171/180 (95%)	169 (99%)	2 (1%)	0	100	100
9	BE	171/180 (95%)	167 (98%)	4 (2%)	0	100	100
10	AF	240/243 (99%)	228 (95%)	12 (5%)	0	100	100
10	BF	240/243 (99%)	230 (96%)	10 (4%)	0	100	100
11	AG	225/236 (95%)	210 (93%)	15 (7%)	0	100	100
11	BG	225/236 (95%)	215 (96%)	10 (4%)	0	100	100
12	AH	121/125 (97%)	116 (96%)	5 (4%)	0	100	100
12	BH	121/125 (97%)	119 (98%)	2 (2%)	0	100	100
13	AI	212/215 (99%)	195 (92%)	16 (8%)	1 (0%)	25	60
13	BI	212/215 (99%)	198 (93%)	13 (6%)	1 (0%)	25	60
14	AJ	127/130 (98%)	111 (87%)	16 (13%)	0	100	100
14	BJ	127/130 (98%)	116 (91%)	11 (9%)	0	100	100
15	AK	122/127 (96%)	117 (96%)	5 (4%)	0	100	100
15	BK	122/127 (96%)	117 (96%)	5 (4%)	0	100	100
16	AL	126/135 (93%)	117 (93%)	9 (7%)	0	100	100
16	BL	126/135 (93%)	119 (94%)	7 (6%)	0	100	100
17	AM	100/102 (98%)	98 (98%)	2 (2%)	0	100	100
17	BM	100/102 (98%)	99 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	AN	125/137 (91%)	119 (95%)	6 (5%)	0	100	100
18	BN	125/137 (91%)	117 (94%)	8 (6%)	0	100	100
19	AO	141/147 (96%)	134 (95%)	7 (5%)	0	100	100
19	BO	141/147 (96%)	138 (98%)	3 (2%)	0	100	100
20	AP	129/148 (87%)	124 (96%)	5 (4%)	0	100	100
20	BP	129/148 (87%)	124 (96%)	5 (4%)	0	100	100
21	AQ	48/56 (86%)	42 (88%)	6 (12%)	0	100	100
21	BQ	48/56 (86%)	43 (90%)	5 (10%)	0	100	100
22	AR	153/158 (97%)	147 (96%)	6 (4%)	0	100	100
22	BR	153/158 (97%)	148 (97%)	5 (3%)	0	100	100
23	AS	108/113 (96%)	103 (95%)	5 (5%)	0	100	100
23	BS	108/113 (96%)	104 (96%)	4 (4%)	0	100	100
24	AT	61/67 (91%)	60 (98%)	1 (2%)	0	100	100
24	BT	61/67 (91%)	59 (97%)	2 (3%)	0	100	100
25	AU	113/132 (86%)	111 (98%)	2 (2%)	0	100	100
25	BU	113/132 (86%)	109 (96%)	4 (4%)	0	100	100
26	AV	146/150 (97%)	144 (99%)	2 (1%)	0	100	100
26	BV	146/150 (97%)	143 (98%)	3 (2%)	0	100	100
27	AW	91/99 (92%)	90 (99%)	1 (1%)	0	100	100
27	BW	91/99 (92%)	86 (94%)	5 (6%)	0	100	100
28	AX	43/50 (86%)	41 (95%)	2 (5%)	0	100	100
28	BX	43/50 (86%)	40 (93%)	3 (7%)	0	100	100
29	AY	59/63 (94%)	57 (97%)	2 (3%)	0	100	100
29	BY	59/63 (94%)	55 (93%)	4 (7%)	0	100	100
30	AZ	64/71 (90%)	64 (100%)	0	0	100	100
30	BZ	64/71 (90%)	63 (98%)	1 (2%)	0	100	100
All	All	8177/8652 (94%)	7782 (95%)	390 (5%)	5 (0%)	50	80

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A4	4	VAL
13	BI	15	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	AI	15	ILE
3	B3	269	ILE
3	A4	66	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A1	53/53 (100%)	51 (96%)	2 (4%)	28	60
1	B1	53/53 (100%)	51 (96%)	2 (4%)	28	60
2	A2	33/35 (94%)	32 (97%)	1 (3%)	36	66
2	B2	33/35 (94%)	33 (100%)	0	100	100
3	A3	265/273 (97%)	261 (98%)	4 (2%)	60	81
3	A4	259/273 (95%)	253 (98%)	6 (2%)	45	72
3	B3	266/273 (97%)	260 (98%)	6 (2%)	45	72
3	B4	257/273 (94%)	250 (97%)	7 (3%)	40	69
4	A5	99/99 (100%)	98 (99%)	1 (1%)	73	87
4	B5	99/99 (100%)	99 (100%)	0	100	100
6	AB	169/173 (98%)	167 (99%)	2 (1%)	67	85
6	BB	169/173 (98%)	168 (99%)	1 (1%)	84	92
7	AC	153/167 (92%)	149 (97%)	4 (3%)	41	70
7	BC	153/167 (92%)	147 (96%)	6 (4%)	27	60
8	AD	161/171 (94%)	158 (98%)	3 (2%)	52	76
8	BD	161/171 (94%)	155 (96%)	6 (4%)	29	62
9	AE	156/160 (98%)	151 (97%)	5 (3%)	34	65
9	BE	156/160 (98%)	155 (99%)	1 (1%)	84	92
10	AF	212/213 (100%)	205 (97%)	7 (3%)	33	64
10	BF	212/213 (100%)	205 (97%)	7 (3%)	33	64
11	AG	188/197 (95%)	183 (97%)	5 (3%)	40	69

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	BG	188/197 (95%)	182 (97%)	6 (3%)	34	65
12	AH	107/108 (99%)	106 (99%)	1 (1%)	75	89
12	BH	107/108 (99%)	105 (98%)	2 (2%)	52	76
13	AI	183/184 (100%)	174 (95%)	9 (5%)	21	54
13	BI	183/184 (100%)	177 (97%)	6 (3%)	33	64
14	AJ	107/108 (99%)	106 (99%)	1 (1%)	75	89
14	BJ	107/108 (99%)	100 (94%)	7 (6%)	14	45
15	AK	100/103 (97%)	97 (97%)	3 (3%)	36	66
15	BK	100/103 (97%)	98 (98%)	2 (2%)	50	75
16	AL	104/111 (94%)	98 (94%)	6 (6%)	17	49
16	BL	104/111 (94%)	103 (99%)	1 (1%)	73	87
17	AM	91/91 (100%)	88 (97%)	3 (3%)	33	64
17	BM	91/91 (100%)	88 (97%)	3 (3%)	33	64
18	AN	94/104 (90%)	93 (99%)	1 (1%)	70	86
18	BN	94/104 (90%)	93 (99%)	1 (1%)	70	86
19	AO	117/121 (97%)	116 (99%)	1 (1%)	75	89
19	BO	117/121 (97%)	114 (97%)	3 (3%)	41	70
20	AP	108/122 (88%)	108 (100%)	0	100	100
20	BP	108/122 (88%)	102 (94%)	6 (6%)	17	50
21	AQ	42/46 (91%)	41 (98%)	1 (2%)	44	71
21	BQ	42/46 (91%)	40 (95%)	2 (5%)	21	55
22	AR	140/143 (98%)	136 (97%)	4 (3%)	37	67
22	BR	140/143 (98%)	139 (99%)	1 (1%)	81	92
23	AS	99/102 (97%)	97 (98%)	2 (2%)	50	75
23	BS	99/102 (97%)	98 (99%)	1 (1%)	73	87
24	AT	57/61 (93%)	55 (96%)	2 (4%)	31	63
24	BT	57/61 (93%)	55 (96%)	2 (4%)	31	63
25	AU	101/114 (89%)	99 (98%)	2 (2%)	50	75
25	BU	101/114 (89%)	98 (97%)	3 (3%)	36	66
26	AV	125/127 (98%)	122 (98%)	3 (2%)	44	71
26	BV	125/127 (98%)	122 (98%)	3 (2%)	44	71

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
27	AW	84/89 (94%)	79 (94%)	5 (6%)	16 48
27	BW	84/89 (94%)	83 (99%)	1 (1%)	67 85
28	AX	37/41 (90%)	36 (97%)	1 (3%)	40 69
28	BX	37/41 (90%)	36 (97%)	1 (3%)	40 69
29	AY	53/54 (98%)	53 (100%)	0	100 100
29	BY	53/54 (98%)	51 (96%)	2 (4%)	28 60
30	AZ	56/60 (93%)	54 (96%)	2 (4%)	30 62
30	BZ	56/60 (93%)	56 (100%)	0	100 100
All	All	7105/7406 (96%)	6929 (98%)	176 (2%)	43 71

All (176) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A1	4	MET
1	A1	34	GLU
2	A2	25	ARG
3	A3	197	GLU
3	A3	210	SER
3	A3	215	ASP
3	A3	270	PHE
3	A4	71	ARG
3	A4	76	SER
3	A4	113	GLU
3	A4	143	TYR
3	A4	164	LEU
3	A4	253	SER
4	A5	116	MET
6	AB	177	TYR
6	AB	184	SER
7	AC	15	MET
7	AC	23	LYS
7	AC	117	LEU
7	AC	150	TYR
8	AD	108	ASN
8	AD	120	MET
8	AD	169	GLU
9	AE	11	TYR
9	AE	30	MET
9	AE	50	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	AE	76	ARG
9	AE	91	ASP
10	AF	83	PHE
10	AF	110	LEU
10	AF	121	PHE
10	AF	141	ASN
10	AF	179	PHE
10	AF	198	ARG
10	AF	231	PHE
11	AG	8	TYR
11	AG	33	ASP
11	AG	131	TRP
11	AG	181	GLN
11	AG	202	PHE
12	AH	37	GLN
13	AI	3	LYS
13	AI	39	LEU
13	AI	85	PHE
13	AI	94	ASN
13	AI	101	TYR
13	AI	113	GLN
13	AI	140	MET
13	AI	151	ASP
13	AI	195	ASP
14	AJ	86	PHE
15	AK	54	LYS
15	AK	73	ARG
15	AK	87	ARG
16	AL	31	LYS
16	AL	49	LEU
16	AL	98	LYS
16	AL	106	MET
16	AL	118	LYS
16	AL	129	LYS
17	AM	35	SER
17	AM	63	ARG
17	AM	89	ARG
18	AN	61	MET
19	AO	71	LYS
21	AQ	21	CYS
22	AR	4	MET
22	AR	49	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	AR	136	TYR
22	AR	147	ARG
23	AS	71	HIS
23	AS	81	LYS
24	AT	20	TYR
24	AT	62	MET
25	AU	28	PHE
25	AU	114	GLU
26	AV	12	LEU
26	AV	77	TYR
26	AV	142	GLU
27	AW	11	ASN
27	AW	24	TYR
27	AW	44	LEU
27	AW	46	LEU
27	AW	84	GLU
28	AX	38	TRP
30	AZ	23	ASP
30	AZ	35	ARG
1	B1	40	CYS
1	B1	51	LYS
3	B3	113	GLU
3	B3	195	LYS
3	B3	198	TYR
3	B3	235	LEU
3	B3	253	SER
3	B3	270	PHE
3	B4	28	LEU
3	B4	114	GLU
3	B4	143	TYR
3	B4	157	LYS
3	B4	179	MET
3	B4	201	LEU
3	B4	203	ASP
6	BB	33	TYR
7	BC	7	PHE
7	BC	57	ARG
7	BC	114	TYR
7	BC	121	MET
7	BC	150	TYR
7	BC	188	ARG
8	BD	59	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	BD	93	ARG
8	BD	104	ASP
8	BD	120	MET
8	BD	157	PHE
8	BD	172	LYS
9	BE	18	TRP
10	BF	81	TYR
10	BF	141	ASN
10	BF	151	SER
10	BF	179	PHE
10	BF	184	TYR
10	BF	196	LYS
10	BF	231	PHE
11	BG	8	TYR
11	BG	24	MET
11	BG	30	GLN
11	BG	42	TYR
11	BG	169	ASP
11	BG	196	ASN
12	BH	18	GLN
12	BH	50	LEU
13	BI	21	TRP
13	BI	46	HIS
13	BI	55	HIS
13	BI	146	TYR
13	BI	195	ASP
13	BI	199	TYR
14	BJ	46	TYR
14	BJ	54	ASP
14	BJ	55	ASP
14	BJ	78	ARG
14	BJ	111	MET
14	BJ	113	HIS
14	BJ	130	TYR
15	BK	5	GLN
15	BK	68	LYS
16	BL	49	LEU
17	BM	1	MET
17	BM	87	ARG
17	BM	102	SER
18	BN	129	LYS
19	BO	29	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	BO	30	TYR
19	BO	71	LYS
20	BP	22	ARG
20	BP	46	ASP
20	BP	49	MET
20	BP	100	MET
20	BP	107	MET
20	BP	134	ASN
21	BQ	27	TYR
21	BQ	54	LYS
22	BR	104	ASN
23	BS	107	GLU
24	BT	36	GLN
24	BT	60	MET
25	BU	18	ASN
25	BU	19	MET
25	BU	60	LYS
26	BV	50	TRP
26	BV	65	ASP
26	BV	83	ARG
27	BW	43	MET
28	BX	5	TRP
29	BY	8	MET
29	BY	40	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A1	54	ASN
2	A2	29	GLN
10	AF	141	ASN
18	AN	123	HIS
13	BI	38	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	AA	1494/1495 (99%)	322 (21%)	46 (3%)
5	BA	1494/1495 (99%)	317 (21%)	46 (3%)
All	All	2988/2990 (99%)	639 (21%)	92 (3%)

All (639) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	AA	4	C
5	AA	32	A
5	AA	35	G
5	AA	38	G
5	AA	39	U
5	AA	42	G
5	AA	43	A
5	AA	44	C
5	AA	45	U
5	AA	46	A
5	AA	47	A
5	AA	57	G
5	AA	65	G
5	AA	72	C
5	AA	73	U
5	AA	74	U
5	AA	75	C
5	AA	77	G
5	AA	89	G
5	AA	100	A
5	AA	101	G
5	AA	104	A
5	AA	105	C
5	AA	106	A
5	AA	108	G
5	AA	112	G
5	AA	114	A
5	AA	115	A
5	AA	116	C
5	AA	129	G
5	AA	141	C
5	AA	148	C
5	AA	177	A
5	AA	183	A
5	AA	197	A
5	AA	198	A
5	AA	199	A
5	AA	202	G
5	AA	240	U
5	AA	241	U
5	AA	243	G
5	AA	247	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	AA	254	G
5	AA	262	G
5	AA	263	C
5	AA	275	A
5	AA	276	A
5	AA	277	G
5	AA	279	U
5	AA	285	C
5	AA	302	A
5	AA	304	C
5	AA	309	A
5	AA	312	U
5	AA	320	G
5	AA	324	C
5	AA	325	A
5	AA	326	C
5	AA	328	G
5	AA	340	A
5	AA	341	C
5	AA	343	G
5	AA	344	G
5	AA	347	G
5	AA	348	C
5	AA	349	A
5	AA	350	G
5	AA	362	C
5	AA	363	C
5	AA	369	A
5	AA	370	A
5	AA	388	G
5	AA	393	A
5	AA	394	C
5	AA	402	G
5	AA	405	G
5	AA	409	C
5	AA	410	U
5	AA	411	C
5	AA	412	U
5	AA	413	G
5	AA	423	U
5	AA	424	U
5	AA	430	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	AA	431	U
5	AA	432	G
5	AA	433	U
5	AA	434	A
5	AA	436	A
5	AA	438	A
5	AA	439	G
5	AA	448	A
5	AA	449	U
5	AA	450	A
5	AA	457	G
5	AA	459	G
5	AA	460	C
5	AA	461	A
5	AA	462	A
5	AA	463	G
5	AA	464	G
5	AA	465	C
5	AA	470	G
5	AA	471	G
5	AA	472	C
5	AA	474	G
5	AA	478	C
5	AA	485	A
5	AA	486	A
5	AA	487	U
5	AA	500	A
5	AA	509	C
5	AA	525	A
5	AA	526	A
5	AA	529	C
5	AA	530	G
5	AA	541	G
5	AA	549	A
5	AA	560	A
5	AA	585	U
5	AA	586	C
5	AA	587	G
5	AA	588	C
5	AA	596	A
5	AA	606	U
5	AA	607	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	AA	615	G
5	AA	619	A
5	AA	620	G
5	AA	621	G
5	AA	640	U
5	AA	641	A
5	AA	642	G
5	AA	647	G
5	AA	648	A
5	AA	649	A
5	AA	655	A
5	AA	656	U
5	AA	657	A
5	AA	669	A
5	AA	671	C
5	AA	673	C
5	AA	675	A
5	AA	678	G
5	AA	685	G
5	AA	696	G
5	AA	702	G
5	AA	703	U
5	AA	707	A
5	AA	709	G
5	AA	710	G
5	AA	717	C
5	AA	731	A
5	AA	735	A
5	AA	747	U
5	AA	748	A
5	AA	767	U
5	AA	769	A
5	AA	770	A
5	AA	771	G
5	AA	775	G
5	AA	776	C
5	AA	782	A
5	AA	798	U
5	AA	799	C
5	AA	800	G
5	AA	801	A
5	AA	804	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	AA	825	C
5	AA	845	G
5	AA	860	G
5	AA	863	U
5	AA	864	G
5	AA	872	A
5	AA	885	G
5	AA	887	G
5	AA	891	A
5	AA	892	C
5	AA	893	U
5	AA	904	G
5	AA	917	A
5	AA	919	U
5	AA	920	U
5	AA	924	U
5	AA	925	U
5	AA	928	A
5	AA	930	G
5	AA	933	G
5	AA	934	G
5	AA	935	G
5	AA	936	A
5	AA	940	U
5	AA	950	C
5	AA	951	G
5	AA	960	A
5	AA	961	U
5	AA	962	G
5	AA	964	A
5	AA	970	G
5	AA	973	U
5	AA	976	A
5	AA	977	G
5	AA	978	G
5	AA	983	G
5	AA	986	G
5	AA	987	G
5	AA	989	C
5	AA	990	G
5	AA	995	G
5	AA	1002	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	AA	1003	G
5	AA	1005	G
5	AA	1007	A
5	AA	1008	U
5	AA	1016	G
5	AA	1017	U
5	AA	1019	A
5	AA	1020	G
5	AA	1022	U
5	AA	1033	G
5	AA	1040	A
5	AA	1046	G
5	AA	1047	U
5	AA	1048	G
5	AA	1053	A
5	AA	1054	A
5	AA	1064	C
5	AA	1070	C
5	AA	1077	U
5	AA	1078	U
5	AA	1081	C
5	AA	1083	G
5	AA	1091	C
5	AA	1096	G
5	AA	1105	C
5	AA	1112	G
5	AA	1118	C
5	AA	1119	U
5	AA	1120	G
5	AA	1128	U
5	AA	1131	G
5	AA	1142	G
5	AA	1143	G
5	AA	1144	G
5	AA	1151	A
5	AA	1157	G
5	AA	1159	U
5	AA	1161	A
5	AA	1162	G
5	AA	1172	A
5	AA	1173	A
5	AA	1184	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	AA	1185	A
5	AA	1186	C
5	AA	1187	A
5	AA	1198	A
5	AA	1199	A
5	AA	1200	U
5	AA	1201	G
5	AA	1210	A
5	AA	1213	G
5	AA	1217	C
5	AA	1218	C
5	AA	1230	G
5	AA	1239	A
5	AA	1240	A
5	AA	1242	C
5	AA	1245	C
5	AA	1246	U
5	AA	1247	A
5	AA	1258	C
5	AA	1260	G
5	AA	1261	U
5	AA	1262	U
5	AA	1263	C
5	AA	1265	G
5	AA	1266	A
5	AA	1279	A
5	AA	1280	C
5	AA	1296	U
5	AA	1298	G
5	AA	1305	U
5	AA	1306	A
5	AA	1307	G
5	AA	1308	U
5	AA	1318	U
5	AA	1323	A
5	AA	1324	U
5	AA	1332	C
5	AA	1334	A
5	AA	1338	C
5	AA	1340	U
5	AA	1341	C
5	AA	1342	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	AA	1344	U
5	AA	1345	G
5	AA	1357	C
5	AA	1358	A
5	AA	1360	C
5	AA	1361	G
5	AA	1407	U
5	AA	1408	C
5	AA	1410	G
5	AA	1413	G
5	AA	1424	G
5	AA	1437	G
5	AA	1445	A
5	AA	1447	A
5	AA	1452	G
5	AA	1454	A
5	AA	1457	A
5	AA	1459	G
5	AA	1460	G
5	AA	1461	U
5	AA	1473	A
5	AA	1475	C
5	AA	1484	C
5	AA	1485	G
5	AA	1487	U
5	AA	1488	C
5	AA	1489	A
5	AA	1491	C
5	BA	4	C
5	BA	8	U
5	BA	16	G
5	BA	26	A
5	BA	35	G
5	BA	38	G
5	BA	39	U
5	BA	40	C
5	BA	42	G
5	BA	43	A
5	BA	44	C
5	BA	45	U
5	BA	47	A
5	BA	57	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	BA	59	C
5	BA	65	G
5	BA	73	U
5	BA	74	U
5	BA	75	C
5	BA	89	G
5	BA	95	G
5	BA	100	A
5	BA	104	A
5	BA	105	C
5	BA	106	A
5	BA	112	G
5	BA	114	A
5	BA	115	A
5	BA	116	C
5	BA	141	C
5	BA	156	A
5	BA	158	U
5	BA	166	A
5	BA	177	A
5	BA	183	A
5	BA	197	A
5	BA	199	A
5	BA	227	C
5	BA	236	C
5	BA	240	U
5	BA	241	U
5	BA	243	G
5	BA	246	A
5	BA	247	G
5	BA	254	G
5	BA	260	C
5	BA	262	G
5	BA	263	C
5	BA	266	A
5	BA	276	A
5	BA	277	G
5	BA	285	C
5	BA	297	G
5	BA	317	A
5	BA	320	G
5	BA	324	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	BA	325	A
5	BA	328	G
5	BA	340	A
5	BA	341	C
5	BA	342	G
5	BA	347	G
5	BA	348	C
5	BA	349	A
5	BA	358	G
5	BA	362	C
5	BA	363	C
5	BA	367	G
5	BA	369	A
5	BA	370	A
5	BA	393	A
5	BA	402	G
5	BA	405	G
5	BA	409	C
5	BA	410	U
5	BA	411	C
5	BA	413	G
5	BA	423	U
5	BA	424	U
5	BA	425	C
5	BA	430	G
5	BA	432	G
5	BA	433	U
5	BA	434	A
5	BA	435	A
5	BA	436	A
5	BA	438	A
5	BA	439	G
5	BA	450	A
5	BA	452	G
5	BA	459	G
5	BA	460	C
5	BA	461	A
5	BA	462	A
5	BA	463	G
5	BA	464	G
5	BA	470	G
5	BA	471	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	BA	472	C
5	BA	474	G
5	BA	480	G
5	BA	485	A
5	BA	486	A
5	BA	487	U
5	BA	500	A
5	BA	509	C
5	BA	513	A
5	BA	514	U
5	BA	517	U
5	BA	520	G
5	BA	525	A
5	BA	526	A
5	BA	529	C
5	BA	530	G
5	BA	549	A
5	BA	574	A
5	BA	585	U
5	BA	586	C
5	BA	587	G
5	BA	588	C
5	BA	596	A
5	BA	607	U
5	BA	615	G
5	BA	619	A
5	BA	640	U
5	BA	641	A
5	BA	642	G
5	BA	647	G
5	BA	649	A
5	BA	655	A
5	BA	656	U
5	BA	657	A
5	BA	658	A
5	BA	673	C
5	BA	676	G
5	BA	677	U
5	BA	678	G
5	BA	685	G
5	BA	702	G
5	BA	703	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	BA	704	C
5	BA	706	G
5	BA	709	G
5	BA	731	A
5	BA	735	A
5	BA	746	A
5	BA	747	U
5	BA	748	A
5	BA	767	U
5	BA	770	A
5	BA	771	G
5	BA	773	A
5	BA	775	G
5	BA	782	A
5	BA	794	A
5	BA	799	C
5	BA	800	G
5	BA	801	A
5	BA	802	G
5	BA	804	U
5	BA	825	C
5	BA	845	G
5	BA	847	A
5	BA	860	G
5	BA	872	A
5	BA	884	G
5	BA	885	G
5	BA	892	C
5	BA	893	U
5	BA	895	C
5	BA	904	G
5	BA	917	A
5	BA	918	A
5	BA	919	U
5	BA	920	U
5	BA	924	U
5	BA	925	U
5	BA	928	A
5	BA	930	G
5	BA	933	G
5	BA	934	G
5	BA	935	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	BA	936	A
5	BA	939	C
5	BA	940	U
5	BA	950	C
5	BA	951	G
5	BA	954	G
5	BA	960	A
5	BA	961	U
5	BA	962	G
5	BA	964	A
5	BA	966	G
5	BA	969	A
5	BA	970	G
5	BA	972	C
5	BA	973	U
5	BA	976	A
5	BA	977	G
5	BA	978	G
5	BA	983	G
5	BA	984	C
5	BA	985	C
5	BA	986	G
5	BA	987	G
5	BA	989	C
5	BA	991	C
5	BA	993	C
5	BA	998	A
5	BA	1002	G
5	BA	1005	G
5	BA	1006	C
5	BA	1007	A
5	BA	1017	U
5	BA	1018	C
5	BA	1020	G
5	BA	1033	G
5	BA	1036	G
5	BA	1038	C
5	BA	1046	G
5	BA	1047	U
5	BA	1050	G
5	BA	1053	A
5	BA	1054	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	BA	1061	A
5	BA	1077	U
5	BA	1078	U
5	BA	1081	C
5	BA	1082	A
5	BA	1096	G
5	BA	1105	C
5	BA	1110	U
5	BA	1112	G
5	BA	1117	A
5	BA	1118	C
5	BA	1119	U
5	BA	1128	U
5	BA	1141	G
5	BA	1142	G
5	BA	1143	G
5	BA	1144	G
5	BA	1156	A
5	BA	1157	G
5	BA	1160	C
5	BA	1161	A
5	BA	1162	G
5	BA	1164	A
5	BA	1171	G
5	BA	1172	A
5	BA	1173	A
5	BA	1174	A
5	BA	1175	C
5	BA	1185	A
5	BA	1186	C
5	BA	1187	A
5	BA	1193	G
5	BA	1198	A
5	BA	1200	U
5	BA	1209	C
5	BA	1218	C
5	BA	1220	G
5	BA	1227	A
5	BA	1228	A
5	BA	1230	G
5	BA	1239	A
5	BA	1240	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	BA	1245	C
5	BA	1246	U
5	BA	1247	A
5	BA	1257	U
5	BA	1258	C
5	BA	1260	G
5	BA	1261	U
5	BA	1262	U
5	BA	1263	C
5	BA	1265	G
5	BA	1272	G
5	BA	1279	A
5	BA	1280	C
5	BA	1282	C
5	BA	1287	G
5	BA	1290	U
5	BA	1291	G
5	BA	1292	A
5	BA	1297	G
5	BA	1298	G
5	BA	1306	A
5	BA	1307	G
5	BA	1308	U
5	BA	1313	G
5	BA	1319	C
5	BA	1323	A
5	BA	1324	U
5	BA	1330	G
5	BA	1332	C
5	BA	1337	A
5	BA	1340	U
5	BA	1341	C
5	BA	1344	U
5	BA	1354	A
5	BA	1357	C
5	BA	1358	A
5	BA	1410	G
5	BA	1413	G
5	BA	1424	G
5	BA	1437	G
5	BA	1445	A
5	BA	1454	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	BA	1459	G
5	BA	1460	G
5	BA	1461	U
5	BA	1484	C
5	BA	1485	G
5	BA	1486	A
5	BA	1487	U
5	BA	1489	A
5	BA	1495	U

All (92) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	AA	42	G
5	AA	56	A
5	AA	99	C
5	AA	111	G
5	AA	176	U
5	AA	239	A
5	AA	246	A
5	AA	262	G
5	AA	324	C
5	AA	368	C
5	AA	408	C
5	AA	435	A
5	AA	462	A
5	AA	471	G
5	AA	528	G
5	AA	641	A
5	AA	655	A
5	AA	672	G
5	AA	746	A
5	AA	766	G
5	AA	871	A
5	AA	919	U
5	AA	924	U
5	AA	939	C
5	AA	960	A
5	AA	961	U
5	AA	975	A
5	AA	977	G
5	AA	985	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	AA	1030	U
5	AA	1053	A
5	AA	1150	G
5	AA	1161	A
5	AA	1245	C
5	AA	1260	G
5	AA	1261	U
5	AA	1262	U
5	AA	1265	G
5	AA	1306	A
5	AA	1307	G
5	AA	1340	U
5	AA	1423	A
5	AA	1436	U
5	AA	1453	U
5	AA	1460	G
5	AA	1483	U
5	BA	42	G
5	BA	56	A
5	BA	99	C
5	BA	103	A
5	BA	111	G
5	BA	176	U
5	BA	239	A
5	BA	246	A
5	BA	262	G
5	BA	324	C
5	BA	362	C
5	BA	368	C
5	BA	424	U
5	BA	431	U
5	BA	434	A
5	BA	528	G
5	BA	584	C
5	BA	641	A
5	BA	655	A
5	BA	672	G
5	BA	746	A
5	BA	766	G
5	BA	871	A
5	BA	919	U
5	BA	924	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	BA	960	A
5	BA	975	A
5	BA	977	G
5	BA	1019	A
5	BA	1053	A
5	BA	1076	G
5	BA	1117	A
5	BA	1161	A
5	BA	1245	C
5	BA	1260	G
5	BA	1261	U
5	BA	1262	U
5	BA	1291	G
5	BA	1306	A
5	BA	1307	G
5	BA	1340	U
5	BA	1423	A
5	BA	1436	U
5	BA	1453	U
5	BA	1460	G
5	BA	1483	U

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

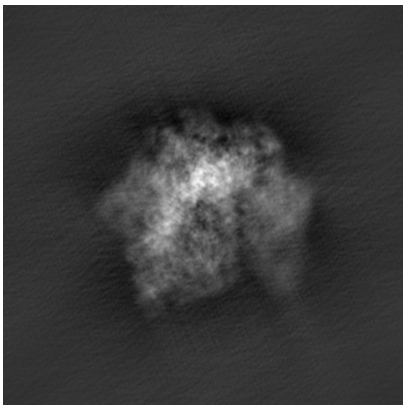
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-50612. These allow visual inspection of the internal detail of the map and identification of artifacts.

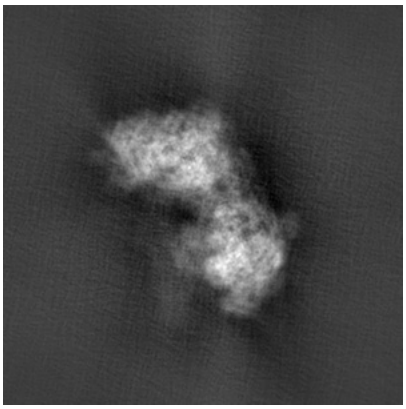
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

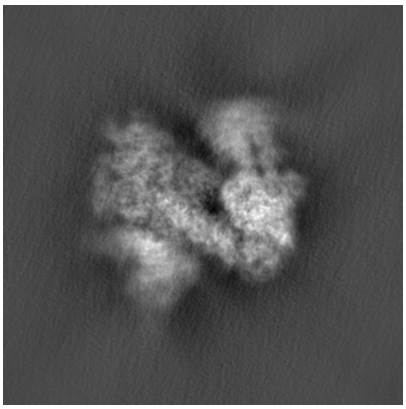
6.1.1 Primary map



X

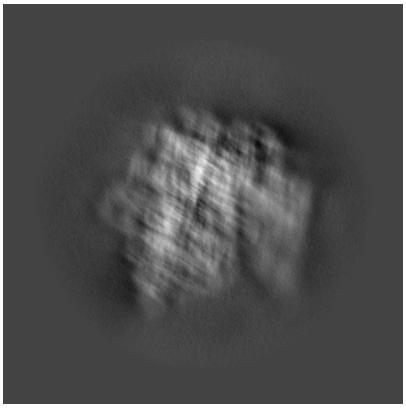


Y

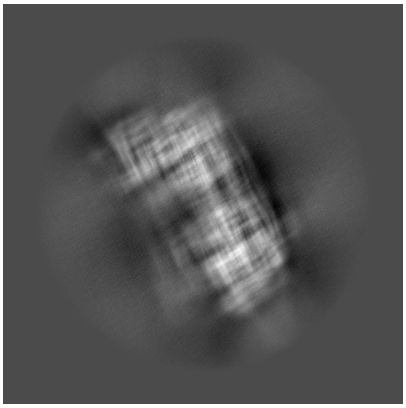


Z

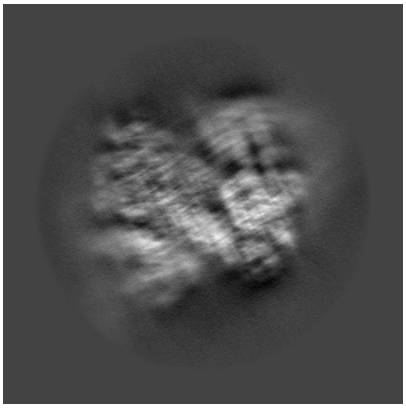
6.1.2 Raw map



X



Y

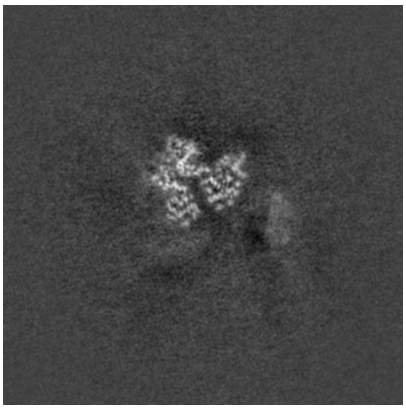


Z

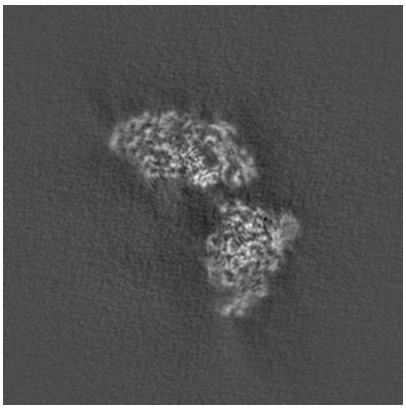
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

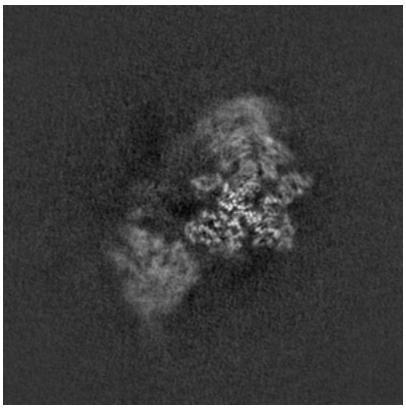
6.2.1 Primary map



X Index: 288

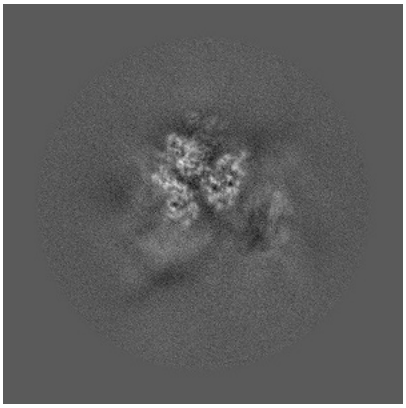


Y Index: 288

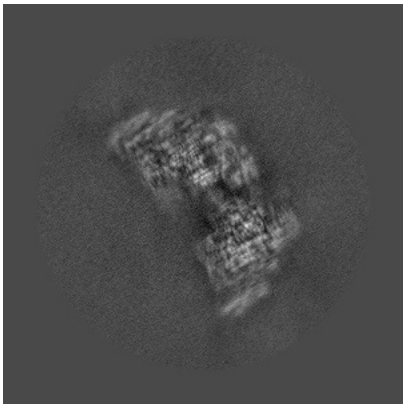


Z Index: 288

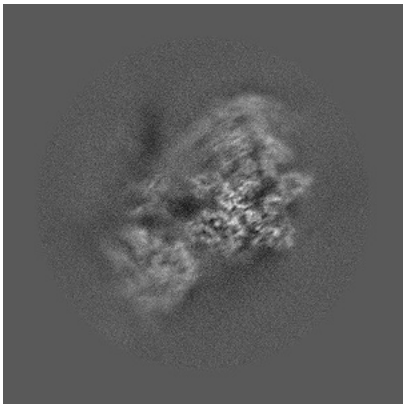
6.2.2 Raw map



X Index: 288



Y Index: 288

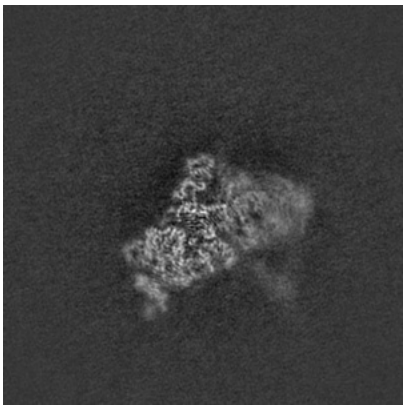


Z Index: 288

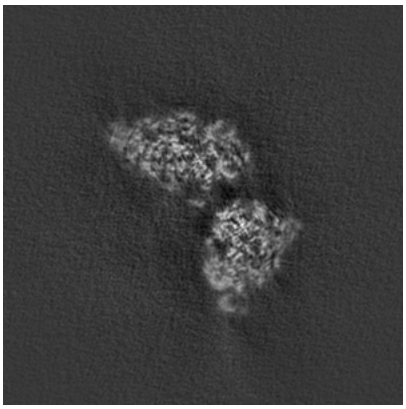
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

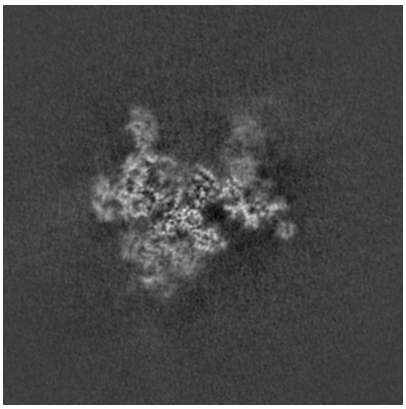
6.3.1 Primary map



X Index: 354

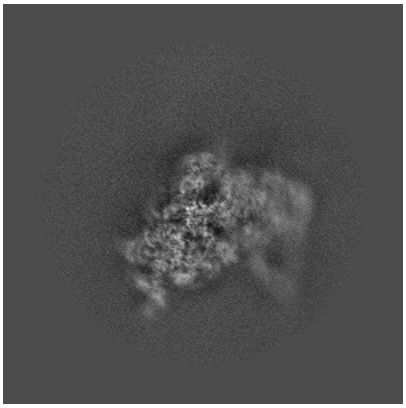


Y Index: 278

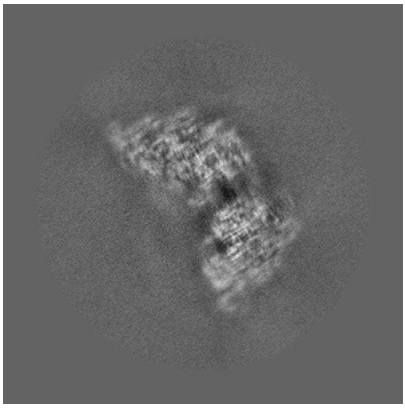


Z Index: 320

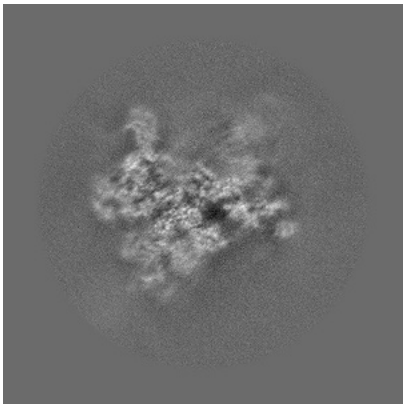
6.3.2 Raw map



X Index: 349



Y Index: 277

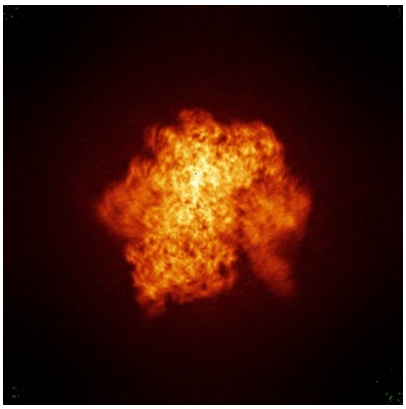


Z Index: 320

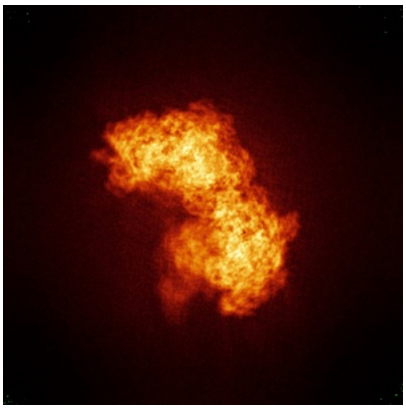
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

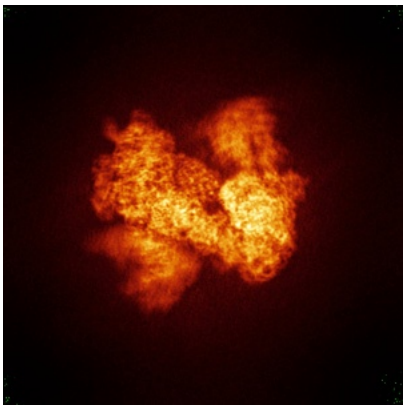
6.4.1 Primary map



X

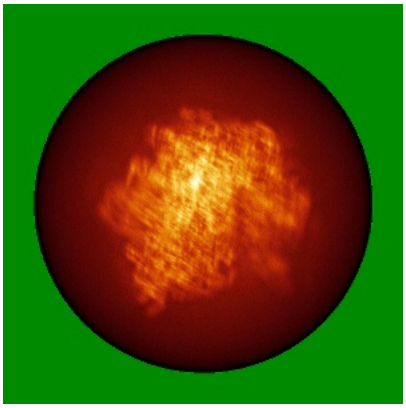


Y

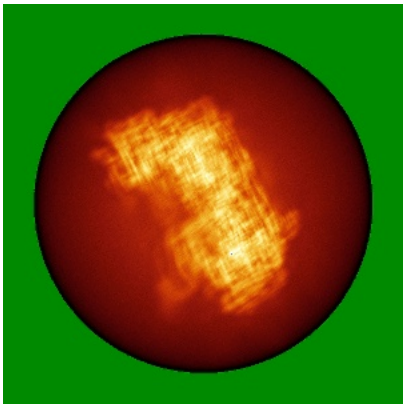


Z

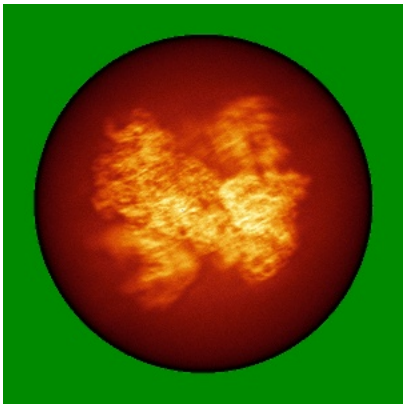
6.4.2 Raw map



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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 3.0. 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

X Y Z

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.

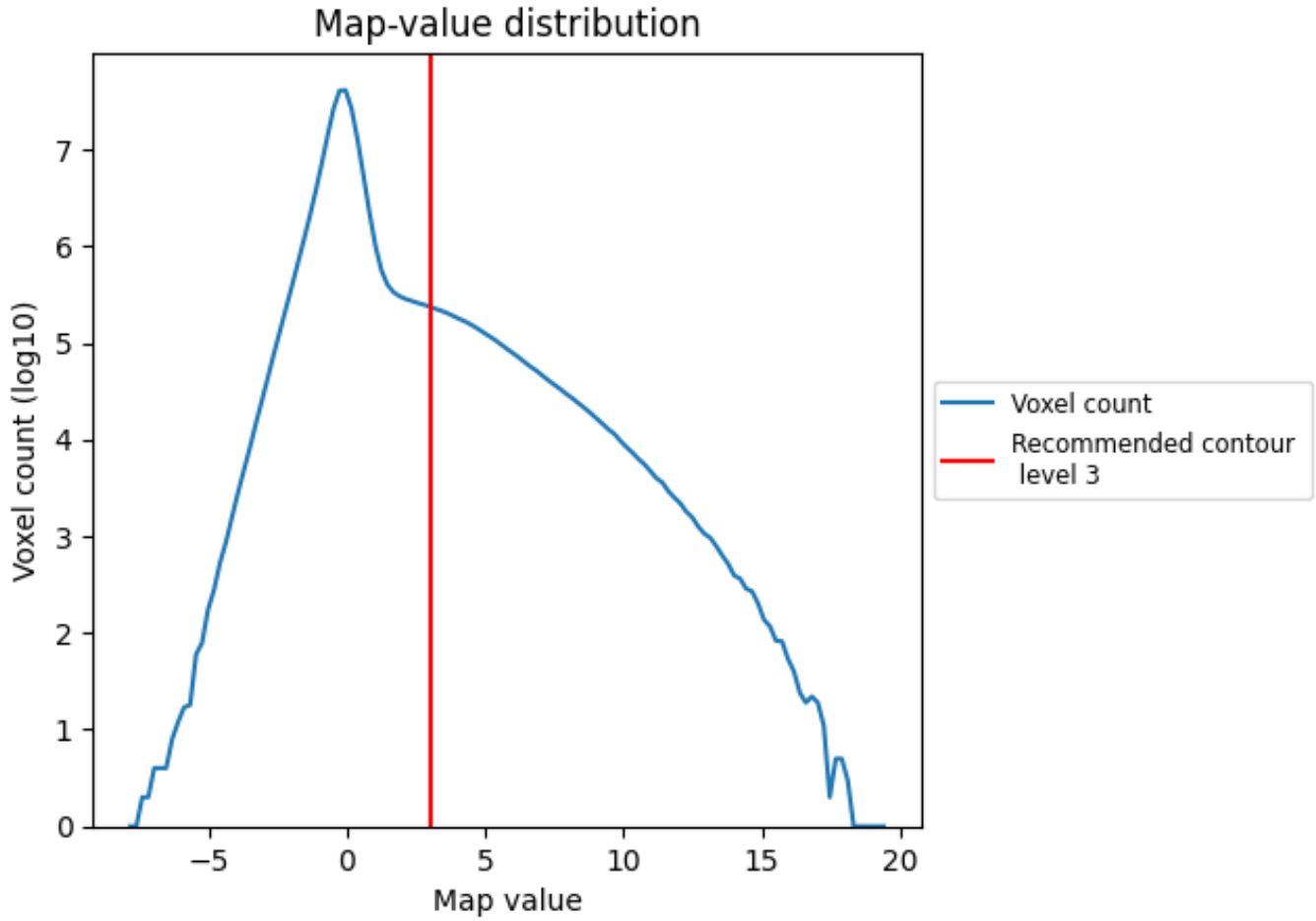
6.6 Mask visualisation (i)

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

7 Map analysis

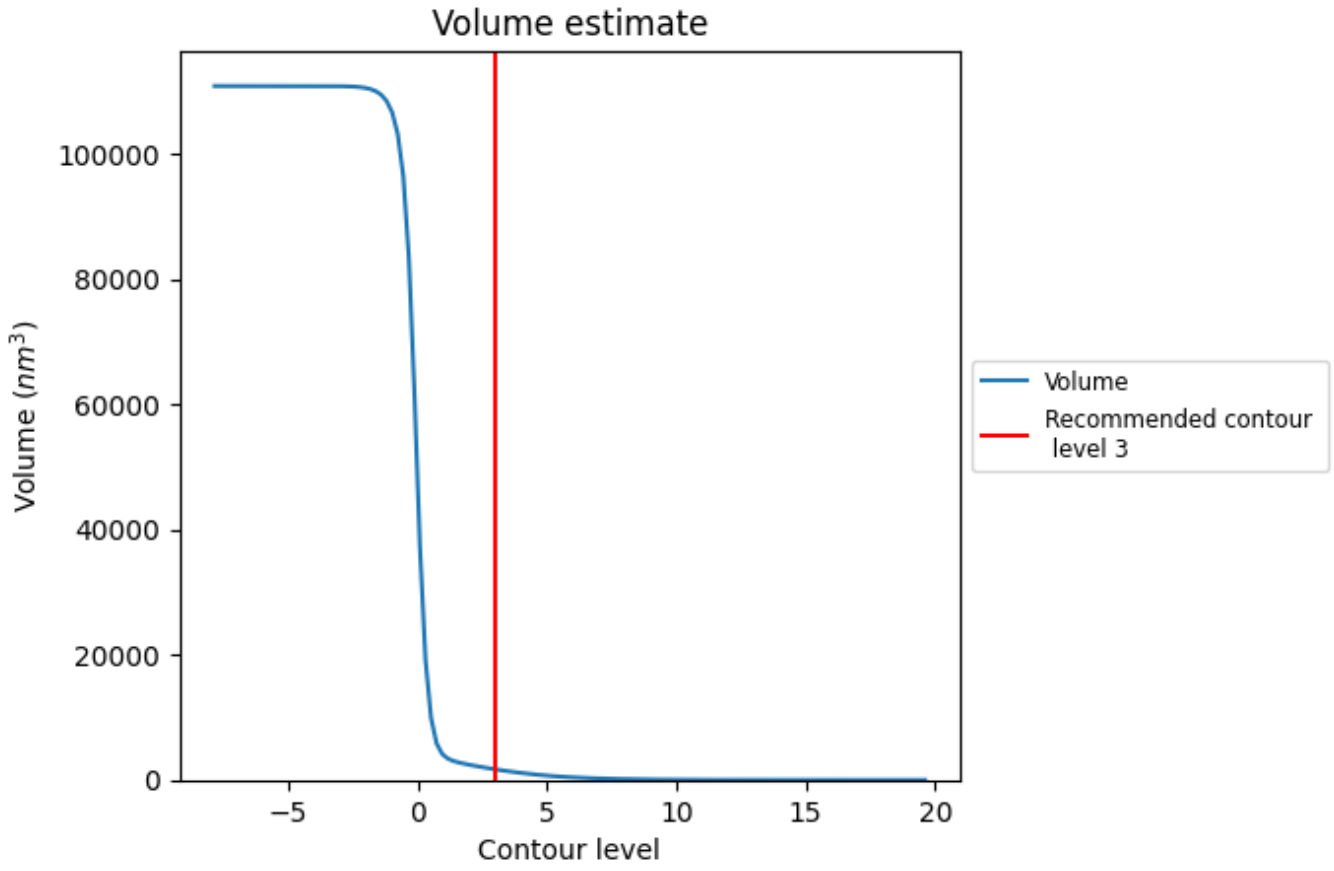
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

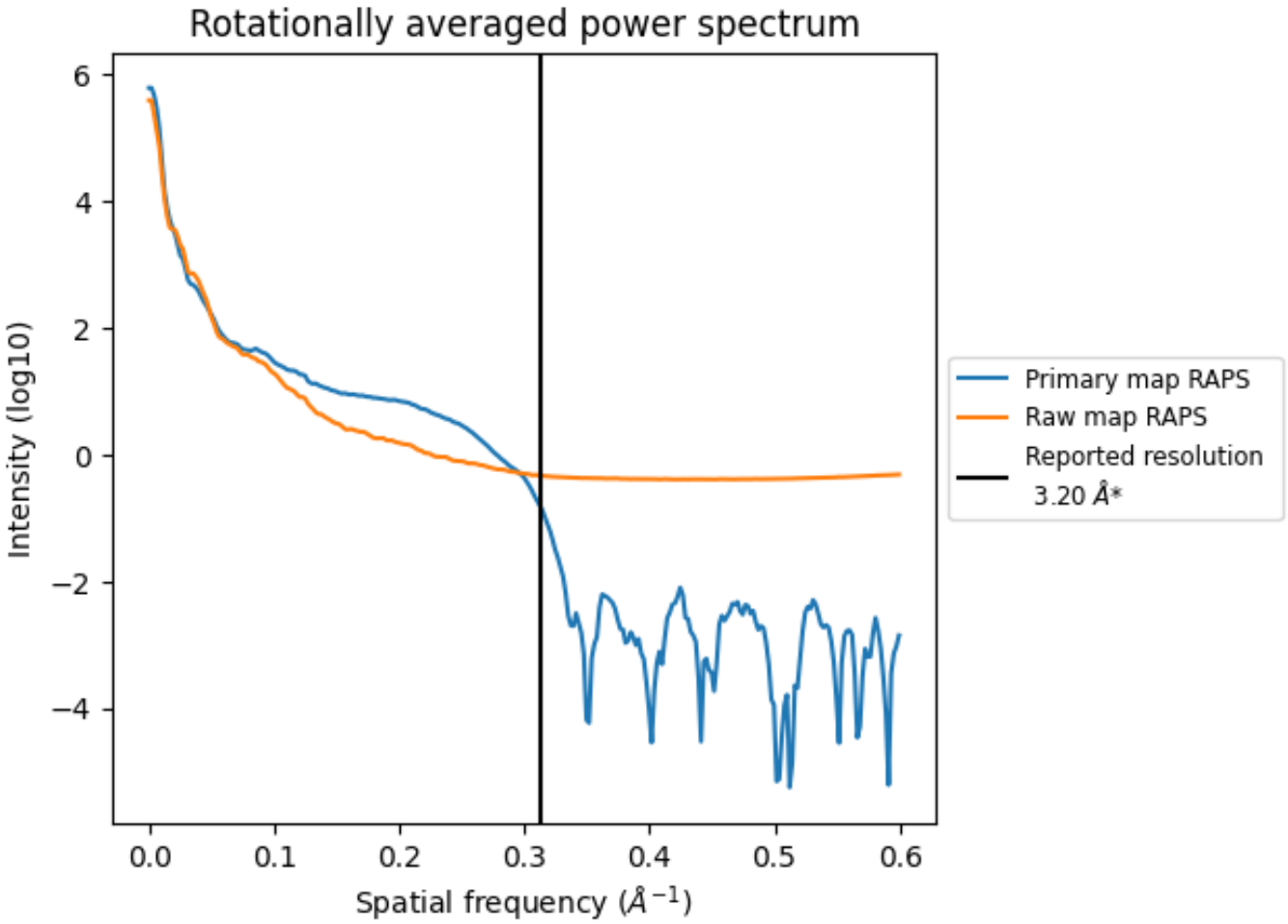
7.2 Volume estimate



The volume at the recommended contour level is 1704 nm^3; this corresponds to an approximate mass of 1539 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 (i)

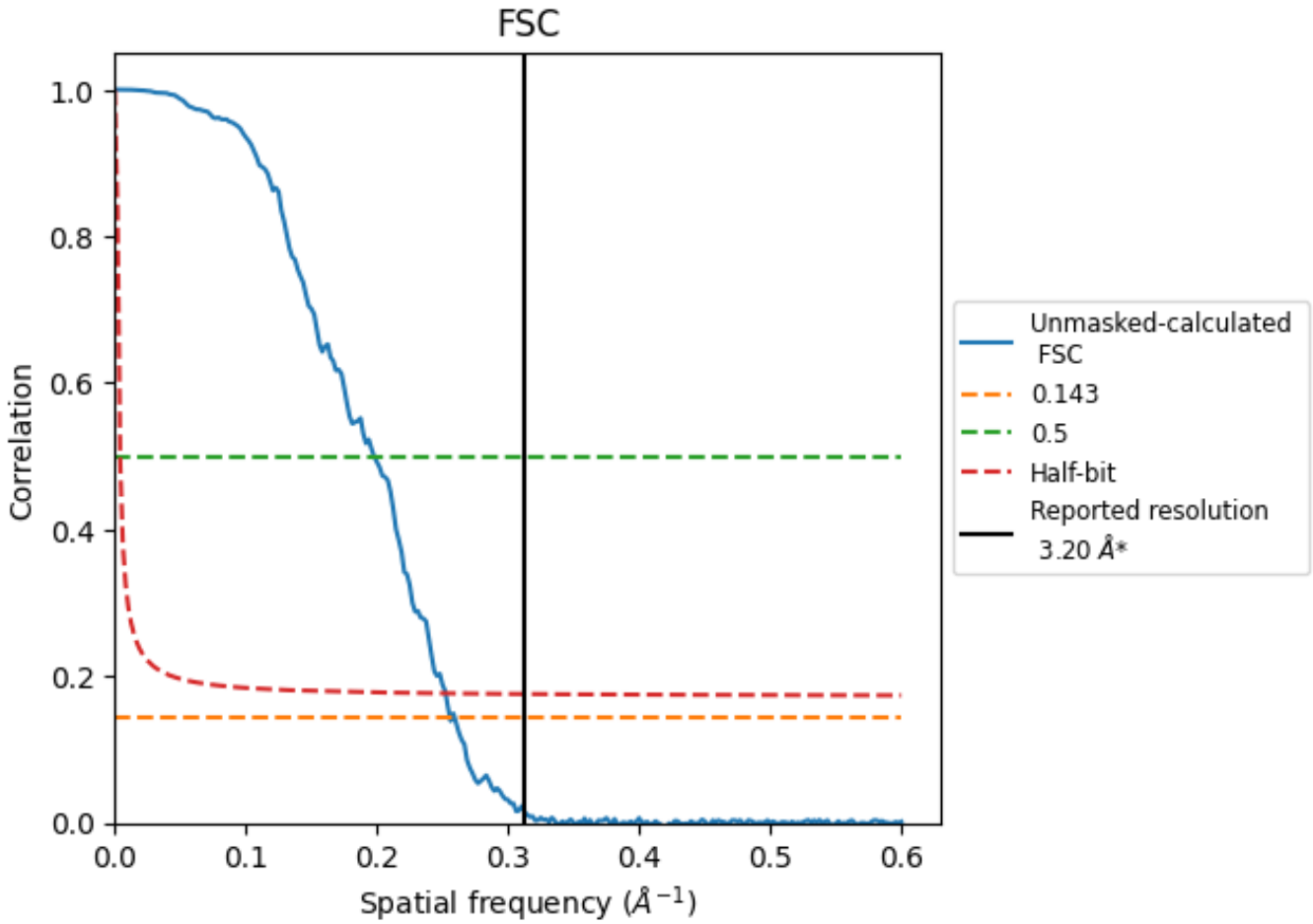


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

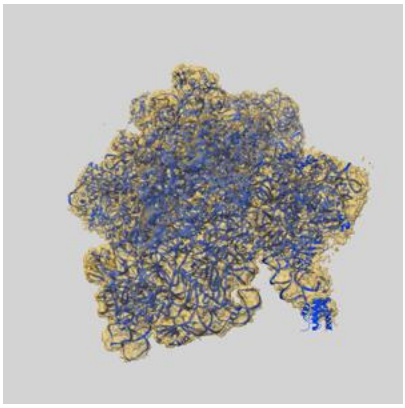
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.91	5.06	3.97

*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 3.91 differs from the reported value 3.2 by more than 10 %

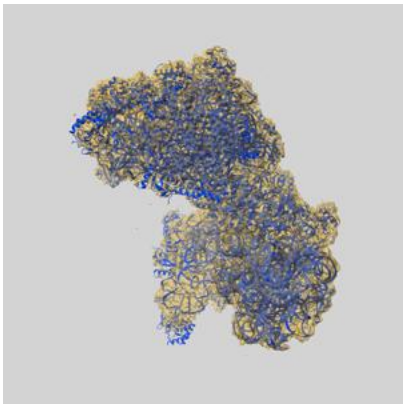
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-50612 and PDB model 9FNZ. Per-residue inclusion information can be found in section 3 on page 13.

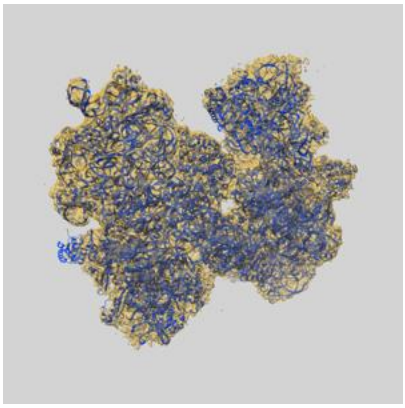
9.1 Map-model overlay



X



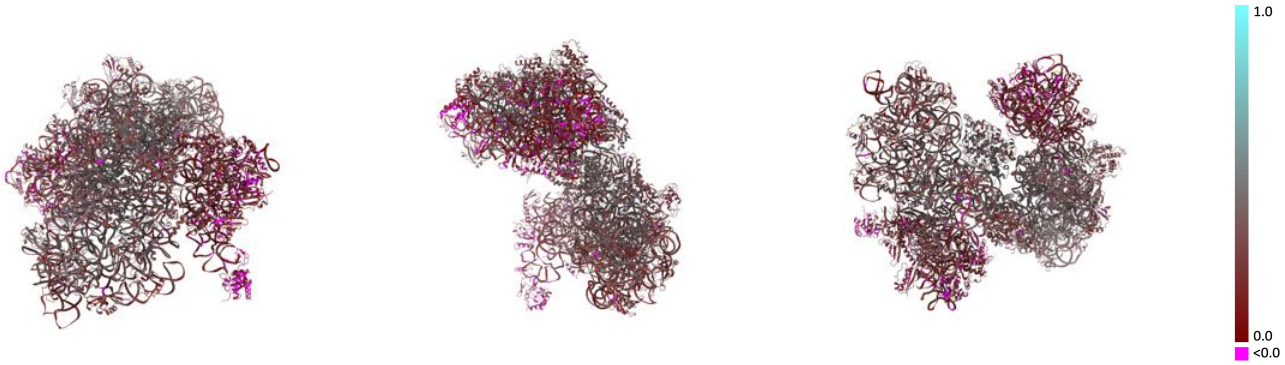
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

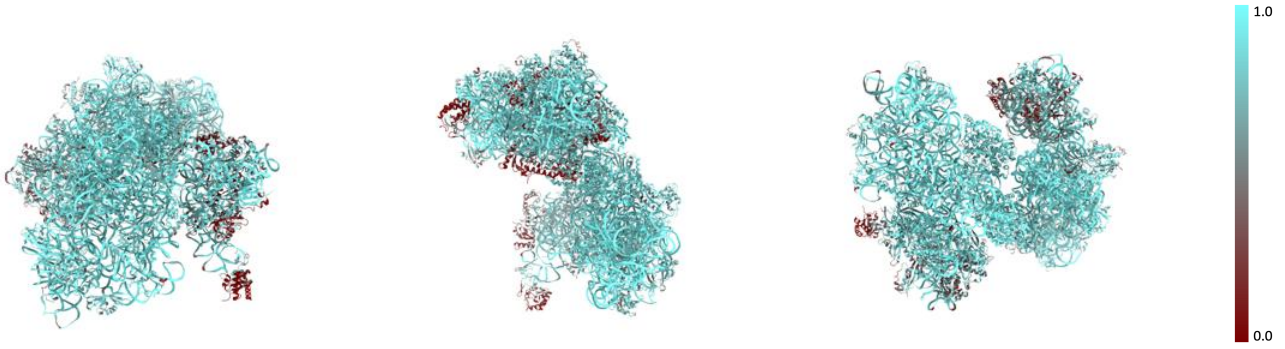
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

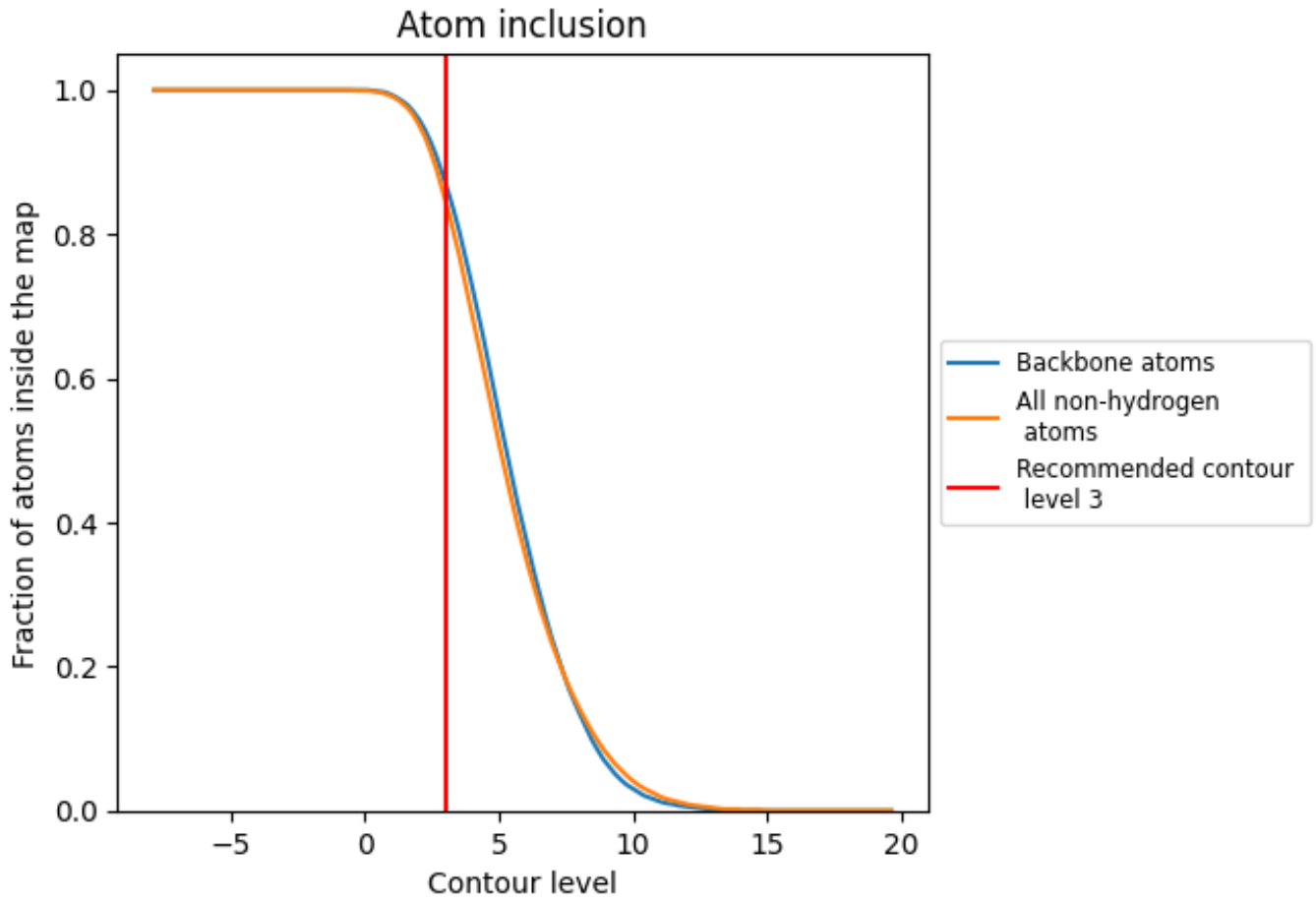
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (3).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8480	0.2880
A1	0.7700	0.3230
A2	0.9160	0.4060
A3	0.8850	0.3810
A4	0.8940	0.3920
A5	0.1290	0.1080
AA	0.9460	0.2950
AB	0.7650	0.3130
AC	0.6690	0.1930
AD	0.8940	0.2980
AE	0.8730	0.3250
AF	0.7950	0.3170
AG	0.8080	0.3530
AH	0.8180	0.3060
AI	0.7490	0.1520
AJ	0.8590	0.3590
AK	0.9140	0.3250
AL	0.6320	0.1520
AM	0.6030	0.1880
AN	0.9630	0.3570
AO	0.8930	0.3520
AP	0.4330	0.1120
AQ	0.7750	0.1940
AR	0.8260	0.3050
AS	0.8430	0.3310
AT	0.7560	0.2600
AU	0.2680	0.1180
AV	0.6120	0.1150
AW	0.7780	0.2880
AX	0.5560	0.0980
AY	0.8880	0.2640
AZ	0.8440	0.2140
B1	0.8240	0.3170
B2	0.8580	0.3730
B3	0.8640	0.3800

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
B4	0.8940	0.3920
B5	0.1660	0.0680
BA	0.9300	0.2990
BB	0.7470	0.2880
BC	0.5240	0.1930
BD	0.8970	0.3500
BE	0.8640	0.3160
BF	0.8350	0.3470
BG	0.8600	0.3490
BH	0.7320	0.2860
BI	0.5460	0.1610
BJ	0.8720	0.3660
BK	0.9150	0.3580
BL	0.7160	0.1490
BM	0.7100	0.1520
BN	0.9730	0.3870
BO	0.9230	0.3680
BP	0.3030	0.1340
BQ	0.6720	0.1430
BR	0.8810	0.3530
BS	0.9110	0.4010
BT	0.8230	0.2370
BU	0.2780	0.1380
BV	0.7570	0.1120
BW	0.7760	0.2710
BX	0.6450	0.0820
BY	0.8470	0.2820
BZ	0.7120	0.1860