Full wwPDB EM Validation Report (i)

Sep 15, 2026 – 01:06 PM EDT

PDB ID	:	7UG7 / pdb_00007ug7
EMDB ID	:	EMD-26486
Title	:	70S ribosome complex in an intermediate state of translocation bound to EF-G(GDP) stalled by Argyrin B
Authors	:	Rundlet, E.J.; Wieland, M.; Holm, M.; Koller, T.O.; Blanchard, S.C.; Wilson, D.N.
Deposited on	:	2022-03-24
Resolution	:	2.58 Å(reported)
Based on initial model	:	7N2C

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 (i) 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 (i)) were used in the production of this report:

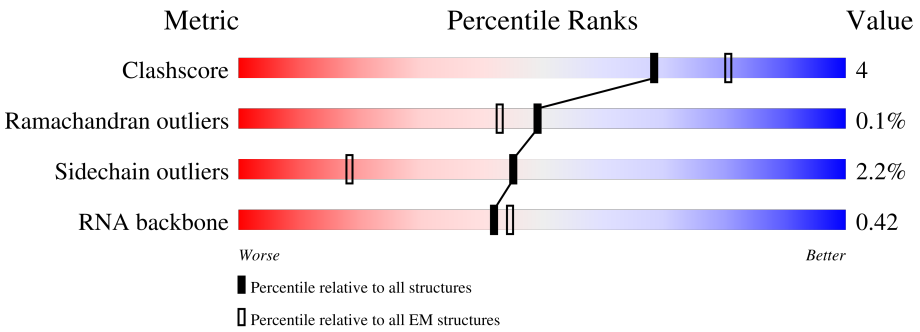
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

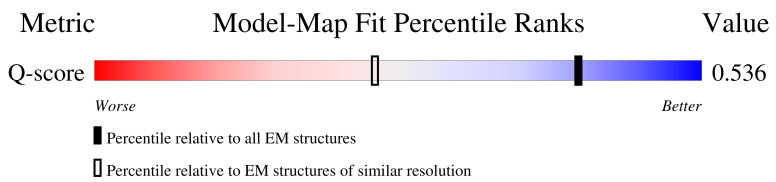
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.58 Å.

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





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7675 (2.08 - 3.08)

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	16	1534	60% 36% • •
2	SB	241	11% 84% 10% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	SC	233	7% 78% 10% 12%
4	SD	206	84% 14%
5	SE	167	78% 14% 7%
6	SF	135	68% 10% 21%
7	SG	179	40% 77% 11% 13%
8	SH	130	88% 11%
9	SI	130	12% 82% 15%
10	SJ	103	16% 77% 18%
11	SK	129	76% 14% 9%
12	SL	124	86% 11%
13	SM	118	25% 81% 16%
14	SN	101	7% 80% 19%
15	SO	89	97%
16	SP	82	88% 12%
17	SQ	84	88% 7% 5%
18	SR	75	75% 15% 11%
19	SS	92	9% 71% 18% 9%
20	ST	87	91% 8%
21	SU	71	6% 89% 10%
22	23	2904	66% 31%
23	5	120	77% 21%
24	LA	234	44% 48% 9% 43%
25	LB	273	93% 6%
26	LC	209	92% 8%
27	LD	201	94% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	LE	179	83% 16%
29	LF	177	86% 12%
30	LI	149	65% 89% 11%
31	LJ	165	65% 66% 12% 22%
32	LK	142	47% 79% 15% 6%
33	LM	142	89% 9%
34	LN	123	88% 11%
35	LO	144	88% 11%
36	LP	136	93% 7%
37	LQ	127	88% 6% 6%
38	LR	117	89% 10%
39	LS	115	93% 6%
40	LT	118	92% 7%
41	LU	103	89% 11%
42	LV	110	93% 7%
43	LW	100	87% 6% 7%
44	LX	104	81% 10% 10%
45	LY	94	91% 9%
46	La	85	87% 6% 7%
47	Lb	78	87% 12%
48	Lc	63	89% 10%
49	Ld	59	92% 7%
50	Le	70	19% 81% 14%
51	Lf	57	81% 16%
52	Lg	55	85% 5% 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	Lh	46	96%
54	Li	65	88% 9%
55	Lj	38	95% 5%
56	EF	700	75% 19%
57	Dt	77	56% 35% 9%
58	Pt	76	45% 43% 8%
59	mR	60	10% 5% 83%
60	B	8	62% 38%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
60	SAR	B	8	-	-	X	-
67	PHE	Pt	3002	-	X	-	-

2 Entry composition (i)

There are 67 unique types of molecules in this entry. The entry contains 154353 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	16	1514	32505	14503	5967	10521	1514	0	0

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	SB	226	1770	1120	317	325	8	0	0

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	SC	206	1624	1028	305	288	3	0	0

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	SD	205	1642	1026	315	297	4	0	0

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	SE	155	1144	711	216	211	6	0	0

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	SF	106	862	545	156	154	7	0	0

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	SG	156	1236	773	238	221	4	0	0

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	SH	129	978	616	173	183	6	0	0

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	SI	127	1021	634	206	178	3	0	0

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	SJ	99	795	498	152	144	1	0	0

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	SK	117	876	540	174	159	3	0	0

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	SL	123	957	591	196	165	5	0	0

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	SM	115	891	552	179	157	3	0	0

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	SN	100	804	499	164	138	3	0	0

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	SO	88	713	439	144	129	1	0	0

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	SP	82	649	406	128	114	1	0	0

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	SQ	80	648	411	121	113	3	0	0

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	SR	67	555	351	106	97	1	0	0

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	SS	84	668	427	127	112	2	0	0

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	ST	86	669	414	138	114	3	0	0

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	SU	70	589	366	125	97	1	0	0

- Molecule 22 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
22	23	2903	62334	27815	11467	20149	2903	0	0

- Molecule 23 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
23	5	120	2570	1144	468	838	120	0	0

- Molecule 24 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	LA	134	1026	645	186	193	2	0	0

- Molecule 25 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	LB	271	2082	1288	423	364	7	0	0

- Molecule 26 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	LC	209	1565	979	288	294	4	0	0

- Molecule 27 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	LD	201	1552	974	283	290	5	0	0

- Molecule 28 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	LE	177	1410	899	249	256	6	0	0

- Molecule 29 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	LF	176	1322	832	243	245	2	0	0

- Molecule 30 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	LI	149	1110	699	197	213	1	0	0

- Molecule 31 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	LJ	129	974	616	173	180	5	0	0

- Molecule 32 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	LK	134	979	619	169	185	6	0	0

- Molecule 33 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	LM	142	1138	720	215	199	4	1	0

- Molecule 34 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	LN	123	946	593	181	166	6	0	0

- Molecule 35 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	LO	144	1063	660	211	190	2	1	0

- Molecule 36 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	LP	136	1074	686	205	177	6	0	0

- Molecule 37 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	LQ	120	960	593	196	166	5	0	0

- Molecule 38 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
38	LR	116	891	552	178	161	0	0

- Molecule 39 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	LS	114	916	574	179	162	1	0	0

- Molecule 40 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
40	LT	117	947	604	192	151	0	0

- Molecule 41 is a protein called Ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	LU	103	815	516	153	144	2	0	0

- Molecule 42 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	LV	110	856	532	166	155	3	0	0

- Molecule 43 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	LW	93	738	466	139	131	2	0	0

- Molecule 44 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
44	LX	94	721	454	136	131	0	0

- Molecule 45 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	LY	94	752	479	137	133	3	0	0

- Molecule 46 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	La	79	595	367	120	107	1	0	0

- Molecule 47 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	Lb	77	624	388	129	105	2	0	0

- Molecule 48 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	Lc	62	501	308	98	94	1	0	0

- Molecule 49 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	Ld	58	448	281	87	78	2	0	0

- Molecule 50 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	Le	67	529	328	100	95	6	0	0

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	Lf	56	444	269	94	80	1	0	0

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
52	Lg	50	409	263	75	71	0	0

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	Lh	46	377	228	90	57	2	0	0

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	Li	64	512	329	107	74	2	1	0

- Molecule 55 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	Lj	38	302	185	65	48	4	0	0

- Molecule 56 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	EF	672	5179	3270	894	992	23	0	0

- Molecule 57 is a RNA chain called tRNA-fMet.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
57	Dt	77	1645	734	298	535	77	1	0	0

- Molecule 58 is a RNA chain called tRNA-Phe.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
58	Pt	76	1637	733	291	535	76	2	0	0

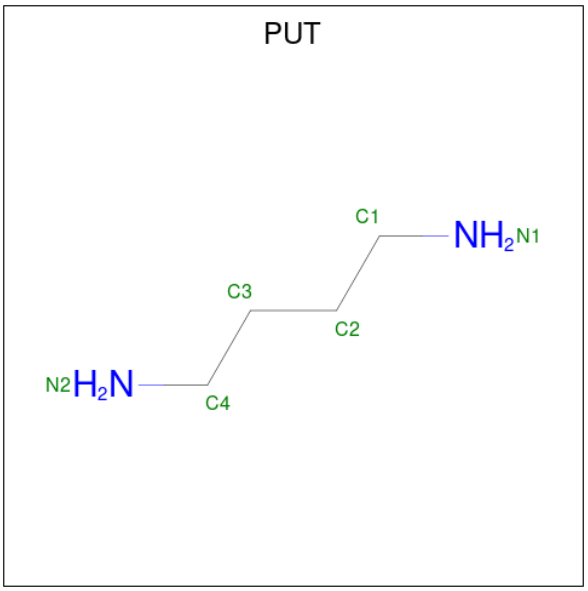
- Molecule 59 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
59	mR	10	214	96	39	69	10	0	0

- Molecule 60 is a protein called Argyrin B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	B	8	60	41	10	8	1	0	0

- Molecule 61 is 1,4-DIAMINOBUTANE (CCD ID: PUT) (formula: $C_4H_{12}N_2$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
61	16	1	6	4	2	0
			Total	C	N	
61	16	1	6	4	2	0
			Total	C	N	
61	23	1	6	4	2	0
			Total	C	N	
61	23	1	6	4	2	0
			Total	C	N	
61	23	1	6	4	2	0
			Total	C	N	
61	23	1	6	4	2	0
			Total	C	N	
61	23	1	6	4	2	0
			Total	C	N	
61	23	1	6	4	2	0
			Total	C	N	
61	23	1	6	4	2	0
			Total	C	N	
61	23	1	6	4	2	0
			Total	C	N	
61	23	1	6	4	2	0

- Molecule 62 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

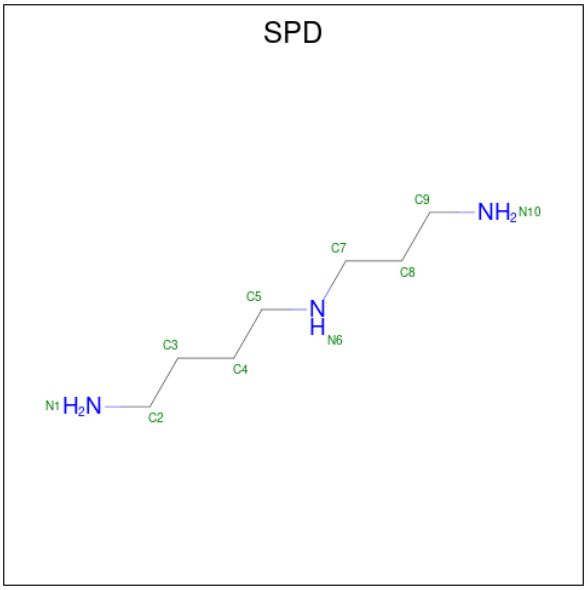
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
62	16	77	77	77	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
62	23	315	315	315	0
			Total	Mg	
62	5	5	5	5	0
			Total	Mg	
62	LB	3	3	3	0
			Total	Mg	
62	LQ	1	1	1	0
			Total	Mg	
62	La	1	1	1	0
			Total	Mg	
62	EF	1	1	1	0
			Total	Mg	
62	Pt	1	1	1	0

- Molecule 63 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).

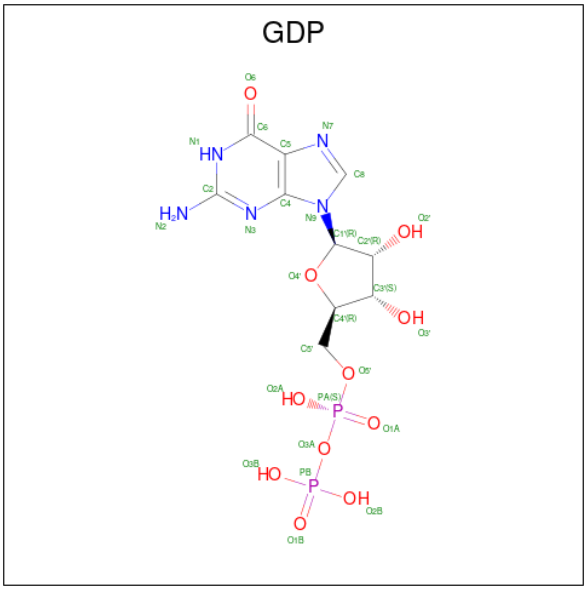


Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
63	23	1	10	7	3	0
			Total	C	N	
63	23	1	10	7	3	0

- Molecule 64 is ZINC ION (CCD ID: ZN) (formula: Zn).

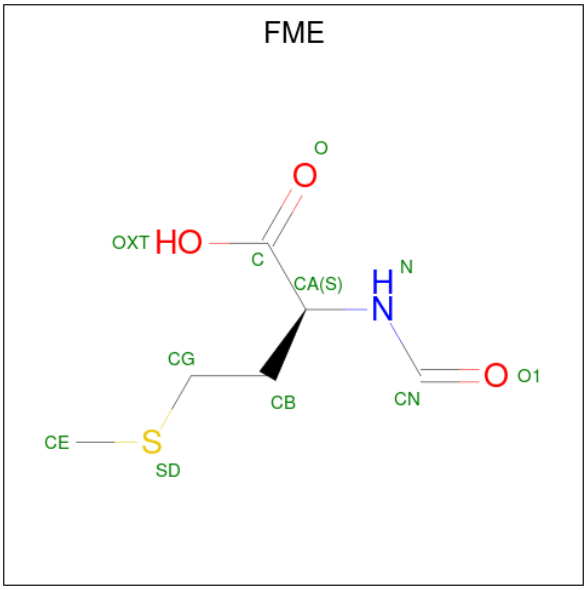
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
64	Le	1	1	1	0
			Total	Zn	
64	Lj	1	1	1	0

- Molecule 65 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



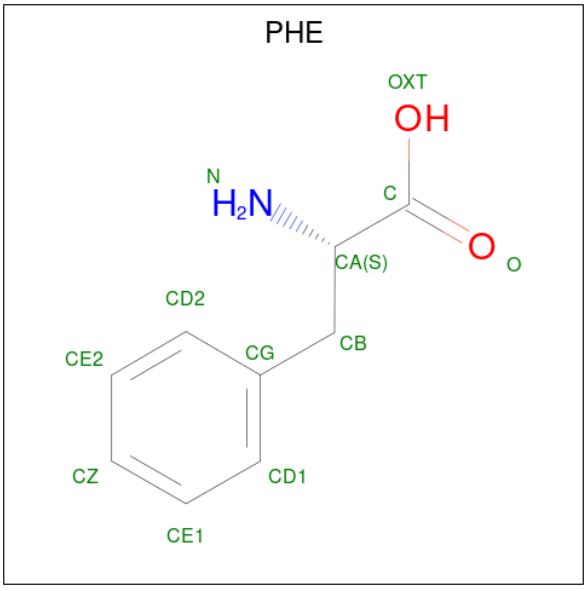
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
65	EF	1	28	10	5	11	2	0

- Molecule 66 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: $C_6H_{11}NO_3S$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
66	Pt	1	10	6	1	2	1	0

- Molecule 67 is PHENYLALANINE (CCD ID: PHE) (formula: $C_9H_{11}NO_2$).



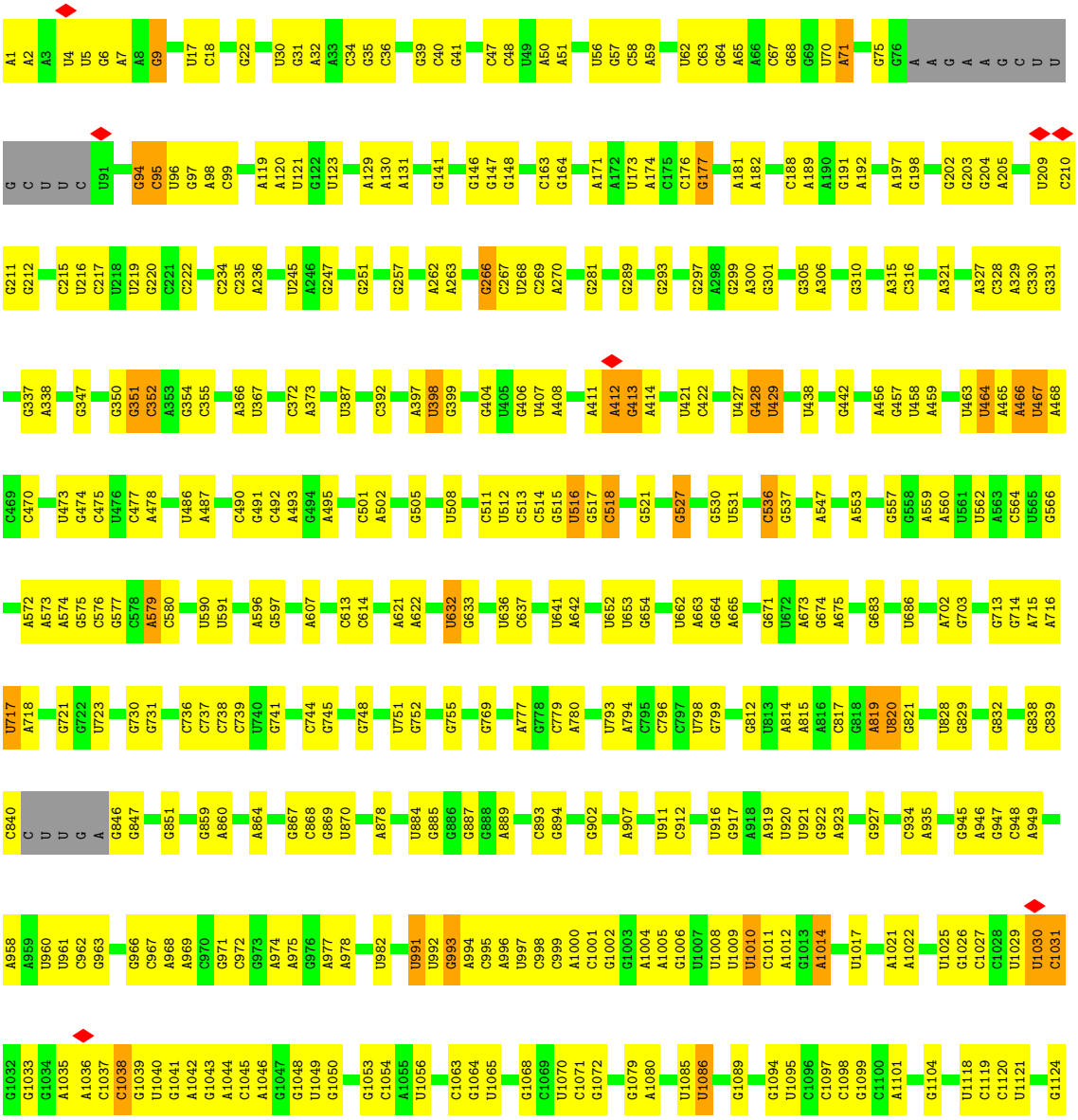
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
67	Pt	1	10	8	1	1	0

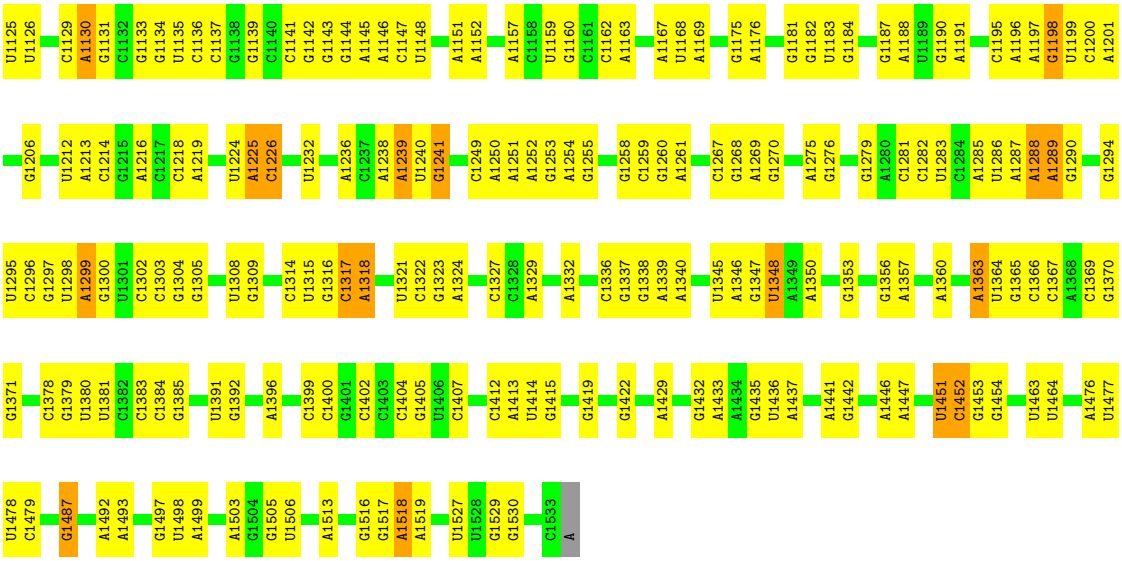
3 Residue-property plots (i)

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: 16S rRNA

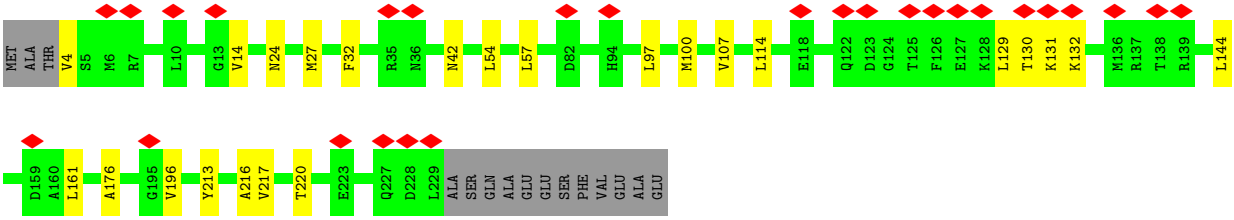
Chain 16: 60% 36%





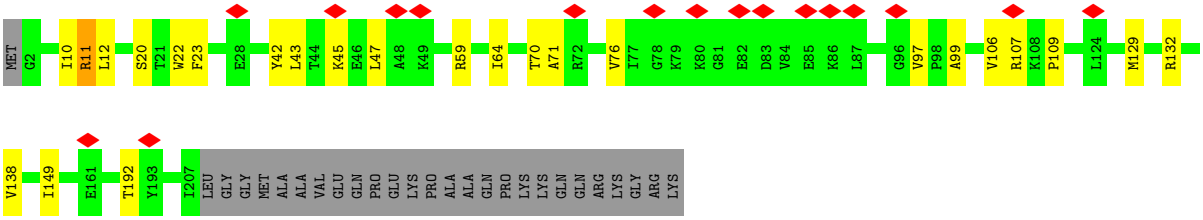
- Molecule 2: 30S ribosomal protein S2

Chain SB:



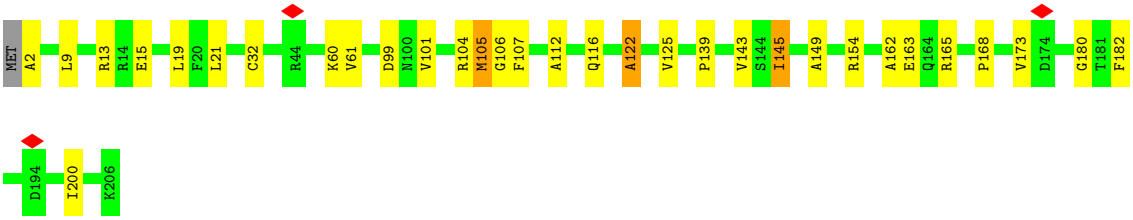
- Molecule 3: 30S ribosomal protein S3

Chain SC:



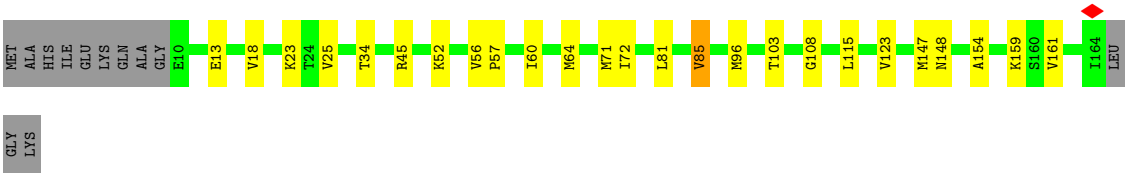
- Molecule 4: 30S ribosomal protein S4

Chain SD:



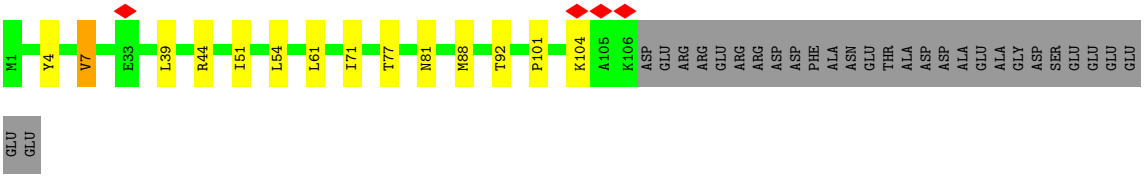
• Molecule 5: 30S ribosomal protein S5

Chain SE:



• Molecule 6: 30S ribosomal protein S6

Chain SF:

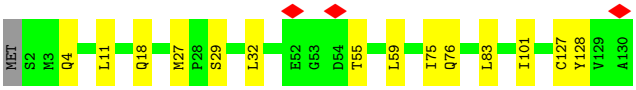


• Molecule 7: 30S ribosomal protein S7

Chain SG:

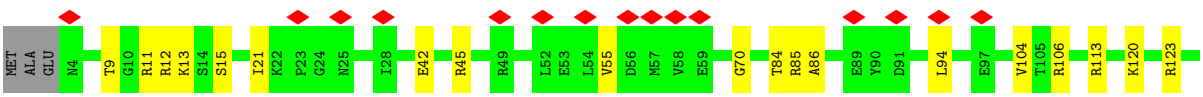
• Molecule 8: 30S ribosomal protein S8

Chain SH:



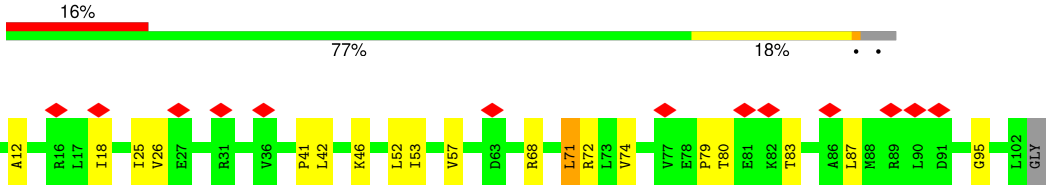
• Molecule 9: 30S ribosomal protein S9

Chain SI:



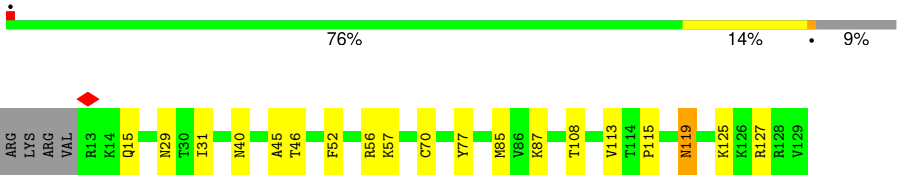
• Molecule 10: 30S ribosomal protein S10

Chain SJ:



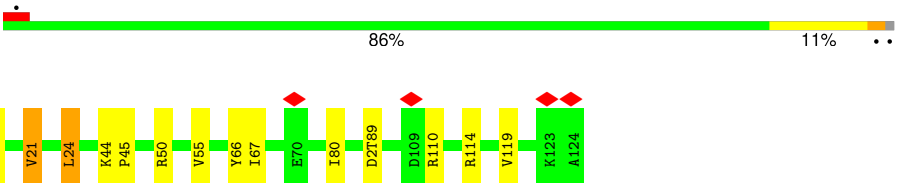
• Molecule 11: 30S ribosomal protein S11

Chain SK:



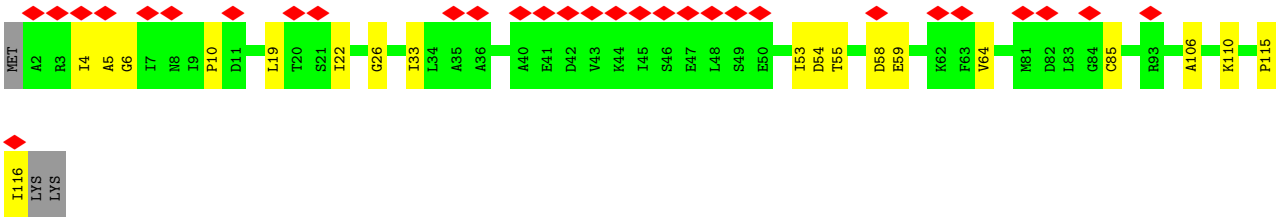
• Molecule 12: 30S ribosomal protein S12

Chain SL:



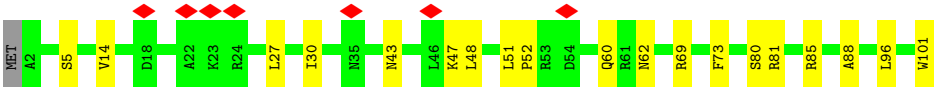
• Molecule 13: 30S ribosomal protein S13

Chain SM:



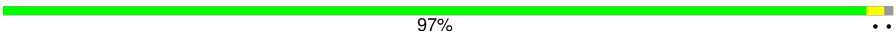
• Molecule 14: 30S ribosomal protein S14

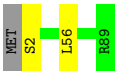
Chain SN:



• Molecule 15: 30S ribosomal protein S15

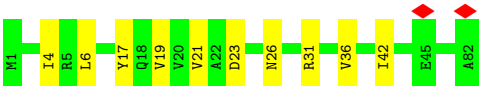
Chain SO:





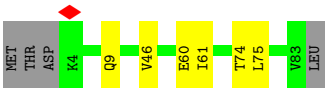
• Molecule 16: 30S ribosomal protein S16

Chain SP:



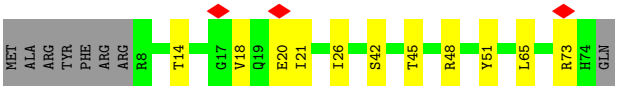
• Molecule 17: 30S ribosomal protein S17

Chain SQ:



• Molecule 18: 30S ribosomal protein S18

Chain SR:

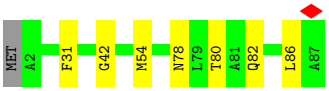


• Molecule 19: 30S ribosomal protein S19

Chain SS:

• Molecule 20: 30S ribosomal protein S20

Chain ST:



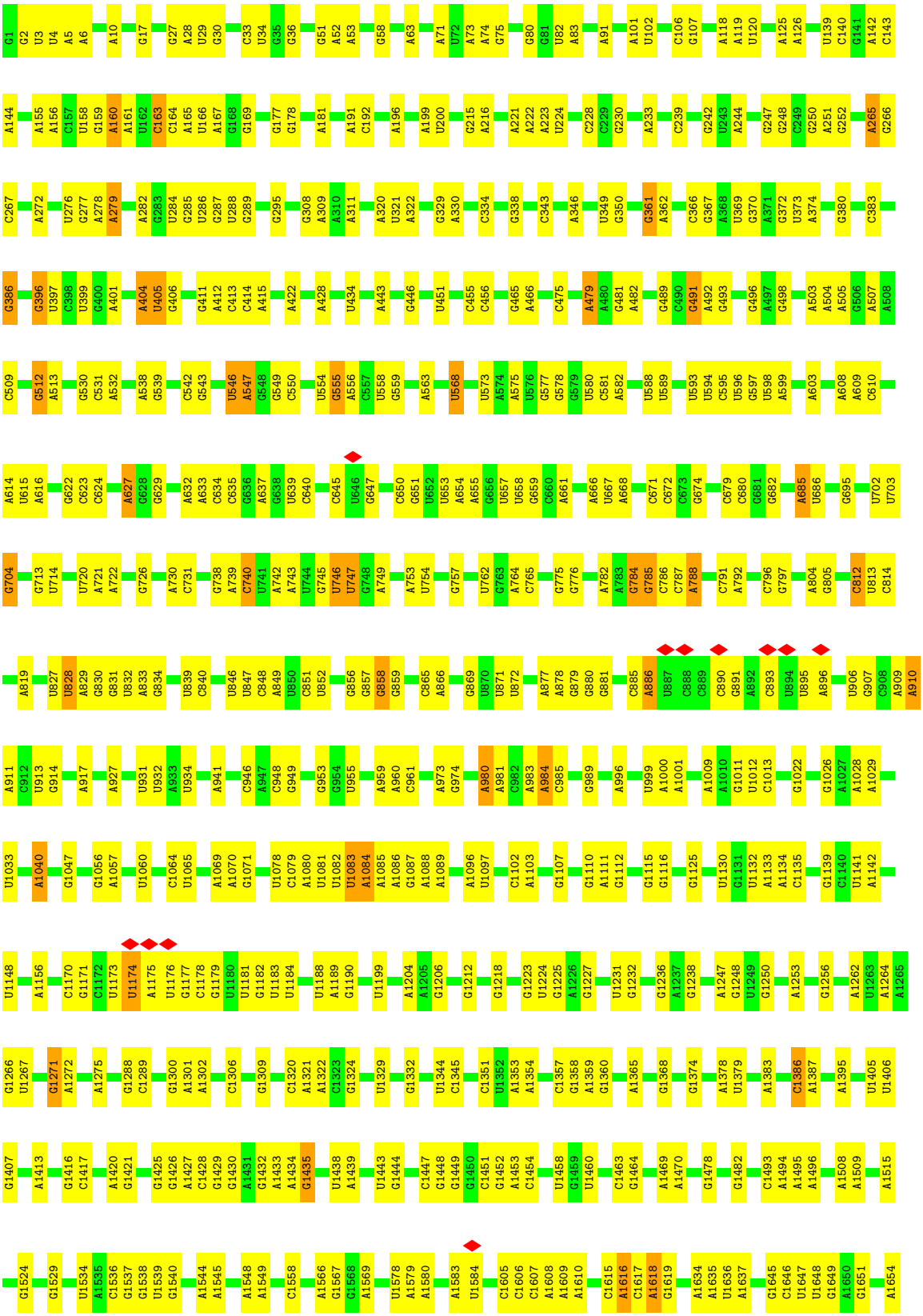
• Molecule 21: 30S ribosomal protein S21

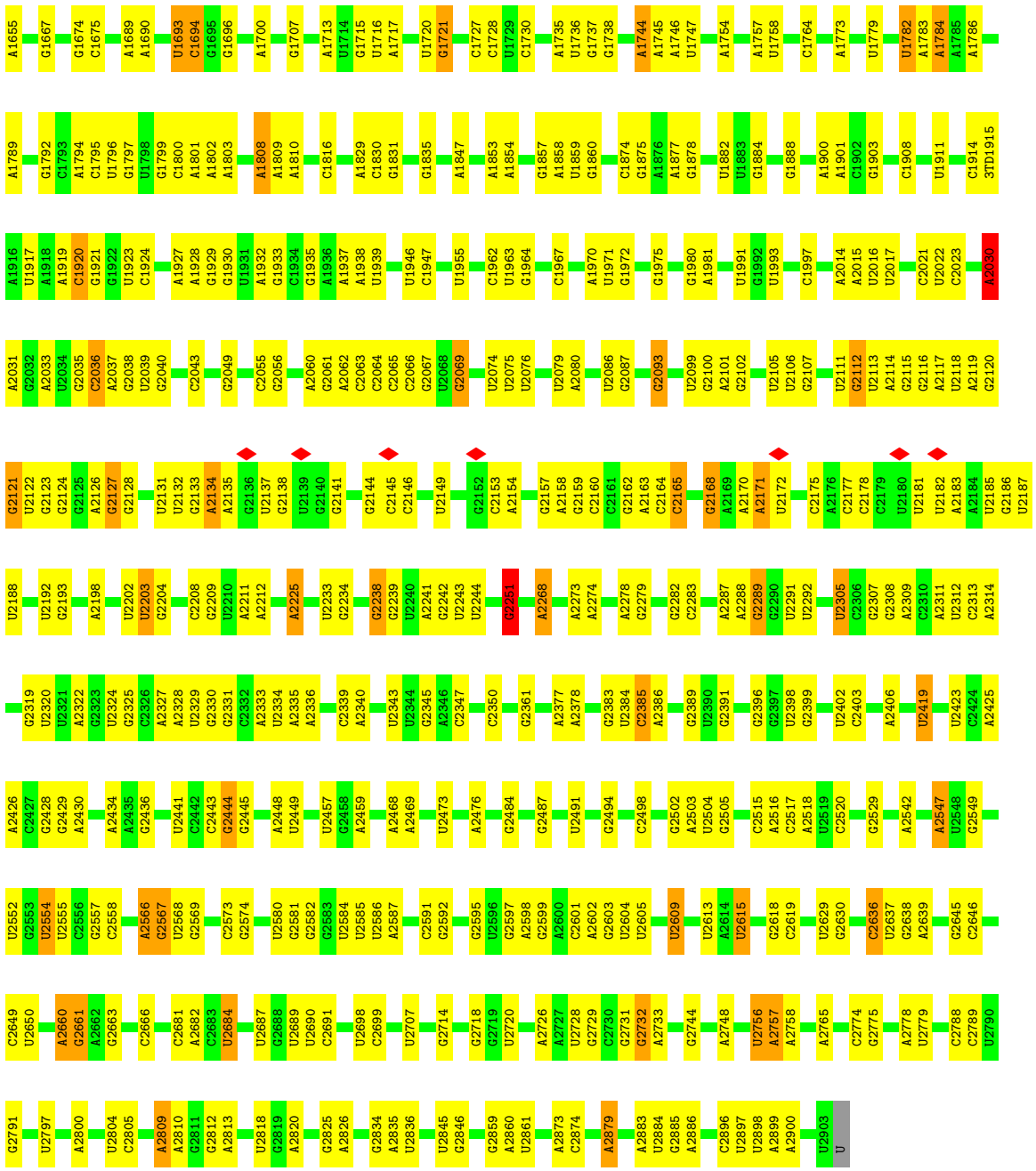
Chain SU:

• Molecule 22: 23S rRNA

Chain 23:

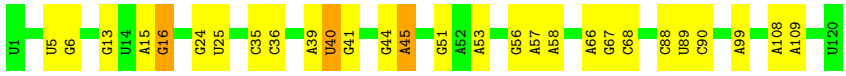
66%
31%


G1 G2 U3 U4 A5 A6 A10 G17 G27 A28 U29 G30 C33 U34 G35 G36 G51 A52 A53 G58 A63 A71 U72 A73 A74 G75 G80 G81 U82 A83 A91 A101 U102 C106 G107 A118 A119 U120 A125 A126 U139 C140 G141 A142 C143
A144 A155 A156 C157 U158 G159 A160 A161 U162 C163 C164 A165 U166 A167 G168 G169 G177 G178 A181 A191 C192 A196 A199 U200 G215 A216 A221 A222 A223 U224 C228 C229 C230 A233 C239 G242 U243 A244 G247 G248 C249 G250 A251 C252 A265 C266
C267 A272 U276 G277 A278 A279 A282 G283 U284 G285 U286 G287 U288 G289 G295 G308 A309 A310 A311 A320 U321 A322 G329 A330 C334 G338 C343 A346 U349 G350 G361 A362 C366 G367 A368 U369 G370 A371 G372 U373 A374 G380 C383
G386 G396 U397 C398 U399 G400 A401 A404 U405 G406 G411 A412 C413 C414 A415 A422 A428 U434 A443 G446 U451 C455 C456 G465 A466 C475 A479 A480 G481 A482 G489 C490 G491 A492 G493 G496 A497 G498 A503 A504 A505 G506 A507 A508
C509 G512 A513 G530 C531 A532 A538 G539 C542 G543 U546 A547 G548 G549 C550 U554 G555 A556 C557 U558 G559 A563 U568 U573 A574 A575 U576 G577 G578 G579 U580 C581 A582 U588 U589 U593 U594 C595 U596 G597 U598 A599 A603 A608 A609 C610
A614 U615 A616 G622 C623 C624 A627 G628 G629 A632 A633 C634 C635 G636 A637 G638 U639 C640 C645 U646 G647 C650 G651 U652 U653 A654 A655 G656 U657 U658 G659 C660 A661 A666 U667 A668 C671 C672 C673 G674 C679 C680 G681 G682 A685 U686 G695 U702 U703
G704 G713 U714 U720 A721 A722 G726 A730 C731 G738 A739 C740 U741 A742 A743 U744 G745 U746 U747 G748 A749 A753 U754 G757 U762 G763 A764 C765 G775 G776 A782 A783 G784 G785 C786 C787 A788 C791 A792 C796 G797 A804 G805 C812 U813 C814
A819 U827 U828 A829 G830 G831 U832 A833 G834 U839 C840 U846 U847 C848 A849 U850 C851 U852 G856 G857 G858 G859 C865 A866 G869 U870 U871 U872 A877 A878 G879 G880 G881 C885 A886 U887 C888 C889 C890 G891 A892 C893 U894 U895 A896 U906 C907 C908 A909 A910
A911 C912 U913 G914 A917 A927 U931 U932 A933 U934 A941 C946 A947 C948 G949 G953 G954 U955 A959 A960 C961 A973 G974 A980 A981 C982 A983 A984 C985 G989 A996 U999 A1000 A1001 A1009 A1010 G1011 U1012 C1013 G1022 G1026 A1027 A1028 A1029
U1033 A1040 G1047 G1056 A1057 U1060 C1064 U1065 A1069 A1070 G1071 U1078 C1079 A1080 U1081 U1082 U1083 A1084 A1085 A1086 G1087 A1088 A1089 A1096 U1097 C1102 A1103 G1107 G1110 A1111 G1112 G1115 G1116 G1125 U1130 G1131 U1132 A1133 A1134 C1135 G1139 C1140 U1141 A1142
U1148 A1156 C1170 G1171 C1172 U1173 U1174 A1175 U1176 G1177 C1178 G1179 U1180 U1181 G1182 U1183 U1184 U1188 A1189 G1190 U1199 A1204 A1205 G1206 G1212 G1218 G1223 U1224 G1225 A1226 G1227 U1231 G1232 G1236 A1237 G1238 A1247 G1248 U1249 G1250 A1253 G1256 A1262 U1263 A1264 A1265
G1266 U1267 G1271 A1272 A1275 G1288 C1289 G1300 A1301 A1302 C1306 G1309 C1320 A1321 A1322 C1323 G1324 U1329 G1332 U1344 C1345 C1351 U1352 A1353 A1354 C1357 G1358 A1359 G1360 A1365 G1368 G1374 A1378 U1379 A1383 C1386 A1387 A1395 U1405 U1406
G1407 A1413 G1416 C1417 A1420 G1421 G1425 G1426 A1427 C1428 G1429 G1430 A1431 G1432 A1433 A1434 G1435 U1438 A1439 U1443 G1444 C1447 G1448 G1449 G1450 C1451 G1452 A1453 C1454 U1458 G1459 U1460 C1463 G1464 A1469 A1470 G1478 G1482 C1493 A1494 A1495 A1496 A1508 A1509 A1515
G1524 G1529 U1534 A1535 C1536 G1537 G1538 U1539 G1540 A1544 A1545 A1548 A1549 C1558 A1566 G1567 C1568 A1569 U1578 A1579 A1580 A1583 U1584 C1605 C1606 C1607 A1608 A1609 A1610 C1615 A1616 C1617 A1618 G1619 A1634 A1635 U1636 A1637 G1645 C1646 U1647 U1648 G1649 A1650 G1651 A1654



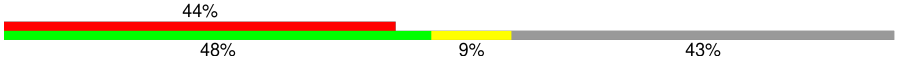
- Molecule 23: 5S rRNA

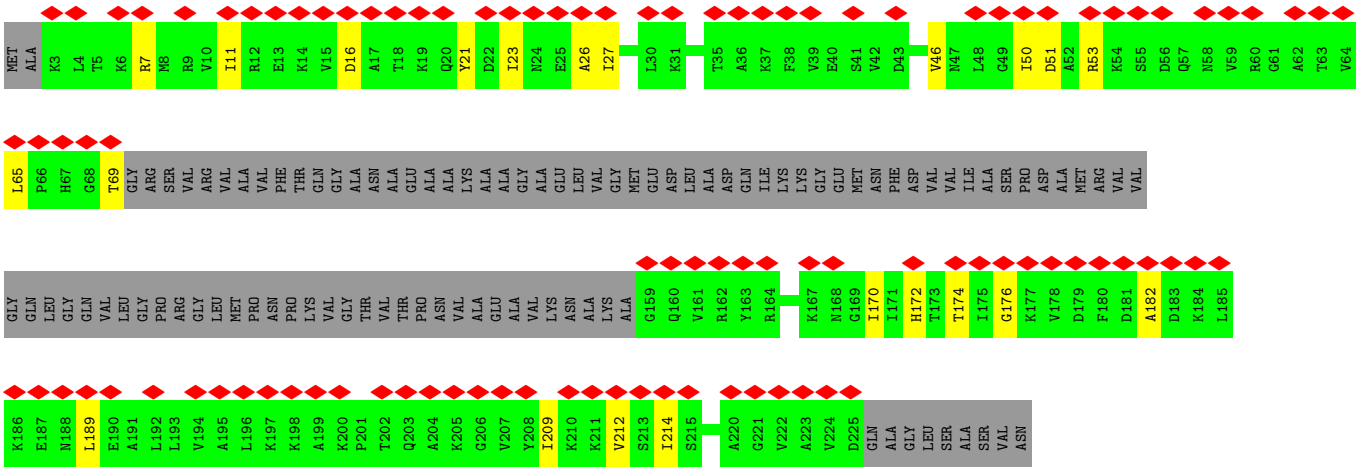
Chain 5:



- Molecule 24: 50S ribosomal protein L1

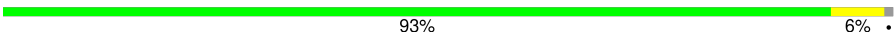
Chain LA:





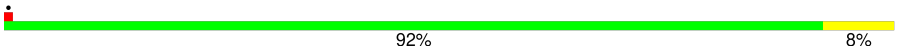
- Molecule 25: 50S ribosomal protein L2

Chain LB:



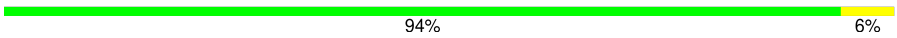
- Molecule 26: 50S ribosomal protein L3

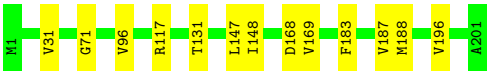
Chain LC:



- Molecule 27: 50S ribosomal protein L4

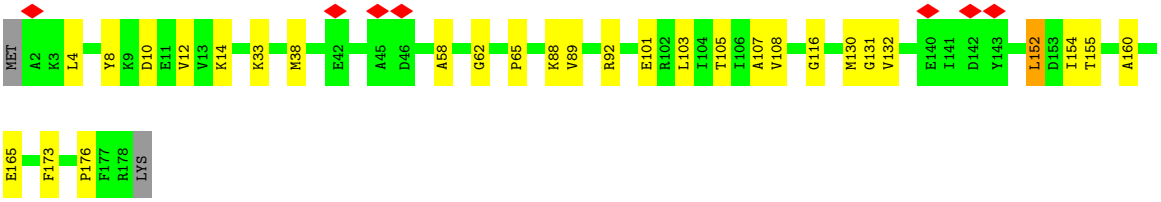
Chain LD:





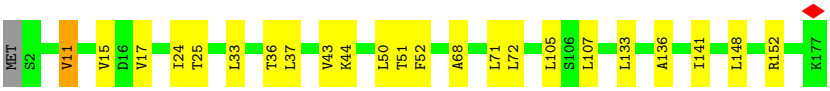
- Molecule 28: 50S ribosomal protein L5

Chain LE:



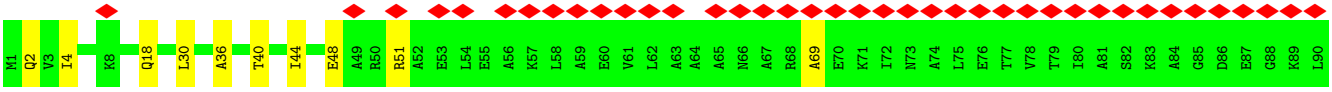
- Molecule 29: 50S ribosomal protein L6

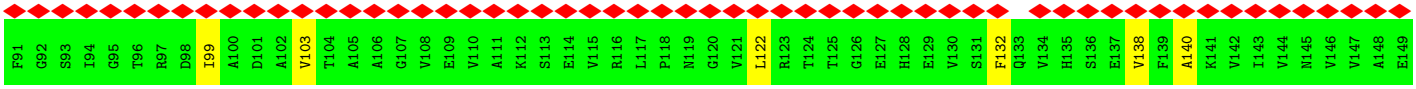
Chain LF:



- Molecule 30: 50S ribosomal protein L9

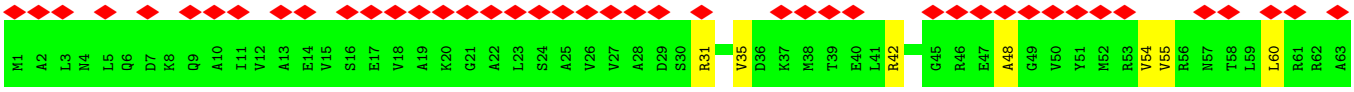
Chain LI:

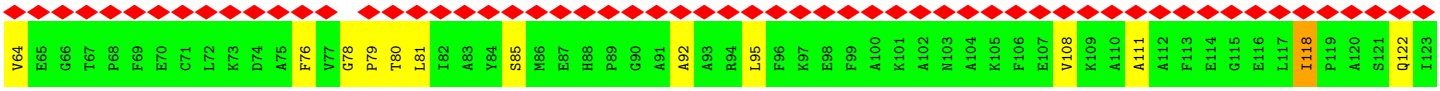


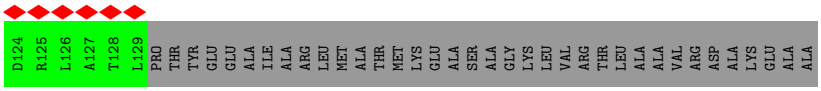


- Molecule 31: 50S ribosomal protein L10

Chain LJ:

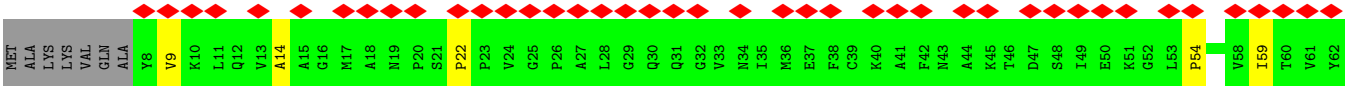


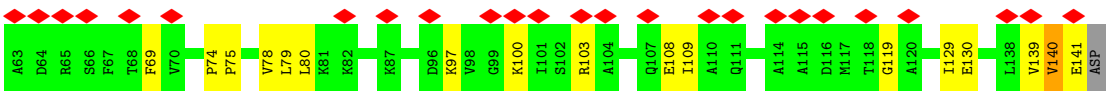




- Molecule 32: 50S ribosomal protein L11

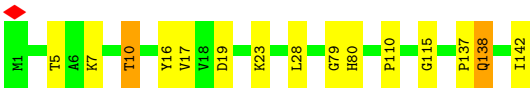
Chain LK:





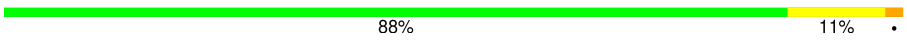
- Molecule 33: 50S ribosomal protein L13

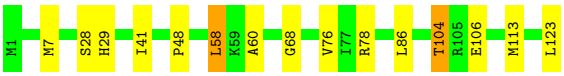
Chain LM:



- Molecule 34: 50S ribosomal protein L14

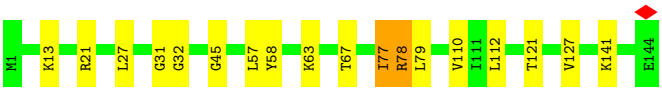
Chain LN:





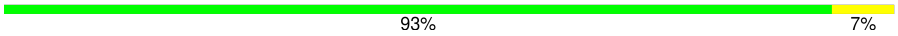
• Molecule 35: 50S ribosomal protein L15

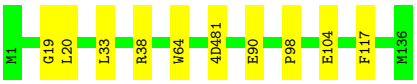
Chain LO:



• Molecule 36: 50S ribosomal protein L16

Chain LP:



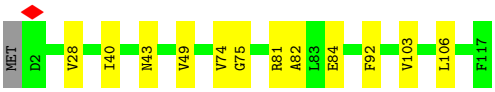


• Molecule 37: 50S ribosomal protein L17

Chain LQ:

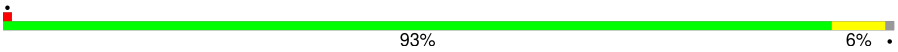
• Molecule 38: 50S ribosomal protein L18

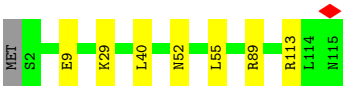
Chain LR:



• Molecule 39: 50S ribosomal protein L19

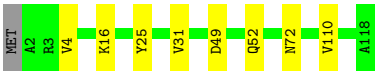
Chain LS:





• Molecule 40: 50S ribosomal protein L20

Chain LT:

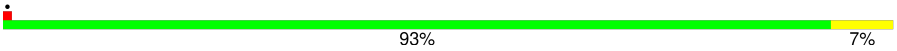


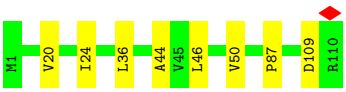
• Molecule 41: Ribosomal protein L21

Chain LU:

• Molecule 42: 50S ribosomal protein L22

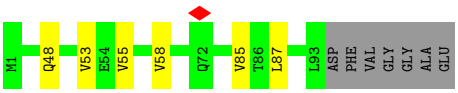
Chain LV:





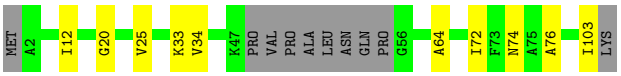
• Molecule 43: 50S ribosomal protein L23

Chain LW:



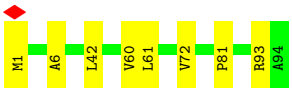
• Molecule 44: 50S ribosomal protein L24

Chain LX:



• Molecule 45: 50S ribosomal protein L25

Chain LY:

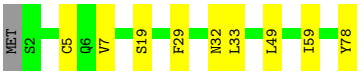


• Molecule 46: 50S ribosomal protein L27

Chain La:

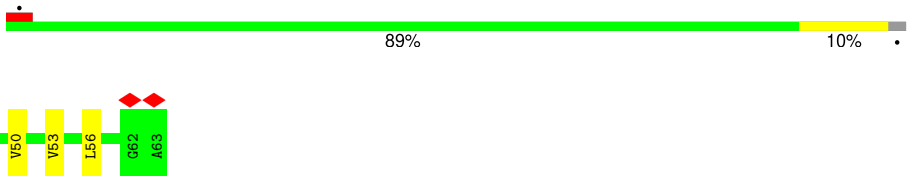
• Molecule 47: 50S ribosomal protein L28

Chain Lb:



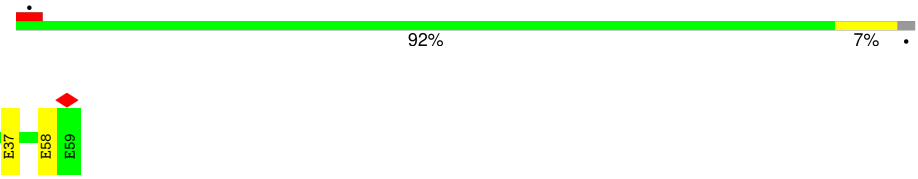
- Molecule 48: 50S ribosomal protein L29

Chain Lc:



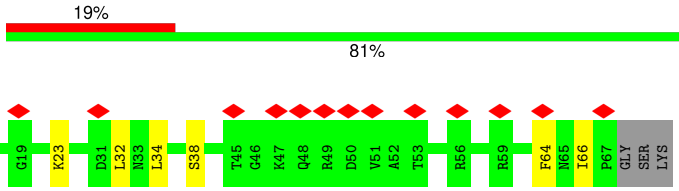
- Molecule 49: 50S ribosomal protein L30

Chain Ld:



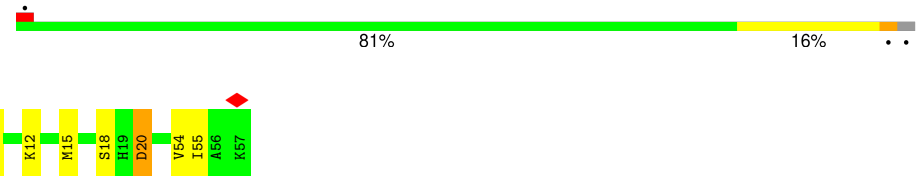
- Molecule 50: 50S ribosomal protein L31

Chain Le:



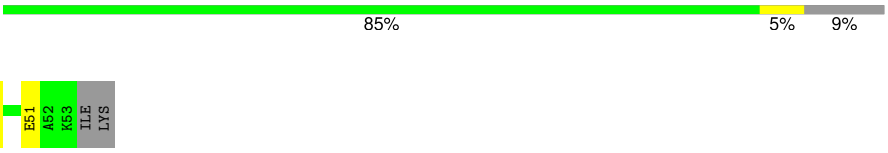
- Molecule 51: 50S ribosomal protein L32

Chain Lf:



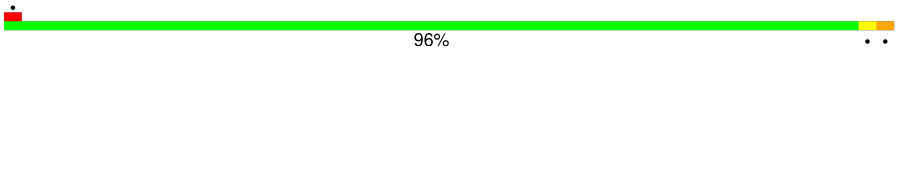
- Molecule 52: 50S ribosomal protein L33

Chain Lg:



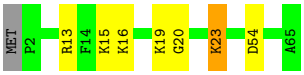
- Molecule 53: 50S ribosomal protein L34

Chain Lh:



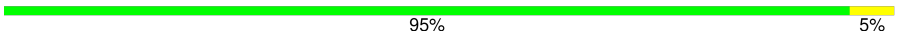
- Molecule 54: 50S ribosomal protein L35

Chain Li:



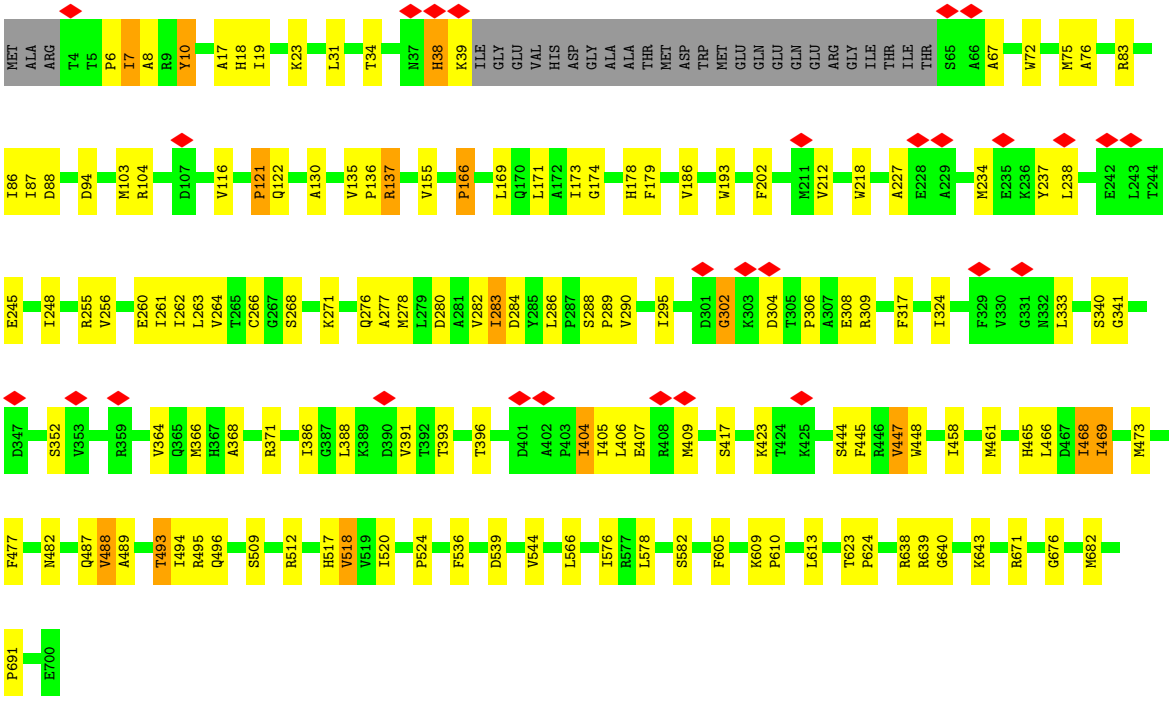
• Molecule 55: 50S ribosomal protein L36

Chain Lj:



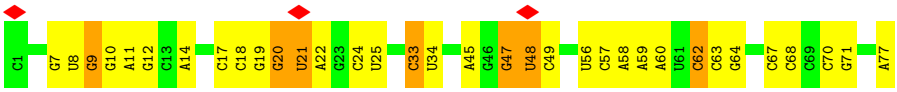
• Molecule 56: Elongation factor G

Chain EF:



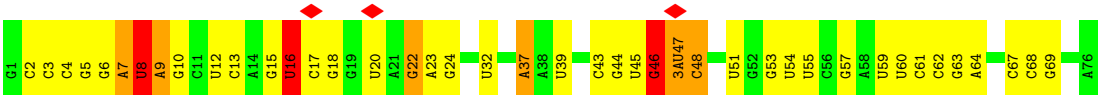
• Molecule 57: tRNA-fMet

Chain Dt:



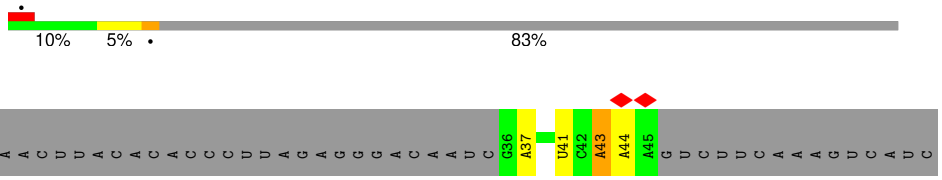
• Molecule 58: tRNA-Phe

Chain Pt:



• Molecule 59: mRNA

Chain mR:



• Molecule 60: Argyrin B

Chain B:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	35220	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 ($e^-/Å^2$)	68	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.070	Depositor
Minimum map value	-0.024	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.007	Depositor
Map size (Å)	400.52002, 400.52002, 400.52002	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.054, 1.054, 1.054	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MA6, 2MA, FME, 1MG, OMU, 3TD, 5MU, PUT, 4SU, 4D4, UR3, PSU, 0UO, 5MC, 6MZ, SPD, BB9, 2MG, OMG, G7M, MG, H2U, MIA, 3AU, DBB, D2T, OMC, DHA, SAR, 4OC, ZN, GDP, DAL

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	16	0.39	0/36143	0.58	0/56376
2	SB	0.87	0/1801	1.11	0/2426
3	SC	0.83	0/1651	1.07	0/2225
4	SD	0.86	0/1664	1.12	0/2227
5	SE	0.95	0/1157	1.22	0/1557
6	SF	0.94	0/881	1.22	0/1189
7	SG	0.68	0/1254	0.93	0/1683
8	SH	0.98	0/988	1.21	1/1326 (0.1%)
9	SI	0.89	0/1033	1.10	0/1375
10	SJ	0.95	0/805	1.16	0/1089
11	SK	0.93	0/892	1.17	0/1205
12	SL	0.95	0/960	1.14	0/1286
13	SM	0.88	0/900	1.12	0/1204
14	SN	0.82	0/816	1.05	0/1088
15	SO	0.82	0/721	1.14	0/964
16	SP	0.90	0/659	1.11	0/884
17	SQ	0.93	0/657	1.13	0/881
18	SR	0.92	0/564	1.19	1/756 (0.1%)
19	SS	0.95	0/685	1.15	0/922
20	ST	0.88	0/675	1.22	0/895
21	SU	0.76	0/597	1.03	0/792
22	23	0.38	1/69239 (0.0%)	0.58	4/108014 (0.0%)
23	5	0.37	0/2873	0.52	0/4478
24	LA	0.88	0/1033	1.08	0/1387
25	LB	0.88	0/2121	1.14	1/2852 (0.0%)
26	LC	0.85	0/1586	1.09	0/2134
27	LD	0.69	0/1571	0.87	0/2113
28	LE	0.90	0/1434	1.15	1/1926 (0.1%)
29	LF	0.84	0/1342	1.05	0/1816
30	LI	0.81	0/1121	1.02	0/1515

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	LJ	0.92	0/986	1.20	0/1328
32	LK	0.94	0/993	1.13	1/1341 (0.1%)
33	LM	0.83	0/1162	1.10	0/1566
34	LN	0.86	0/955	1.10	0/1279
35	LO	0.91	0/1072	1.21	1/1427 (0.1%)
36	LP	0.85	0/1080	1.08	1/1443 (0.1%)
37	LQ	0.69	0/973	0.95	1/1301 (0.1%)
38	LR	0.83	0/901	1.10	0/1209
39	LS	0.79	0/928	1.02	0/1242
40	LT	0.73	0/960	1.02	0/1278
41	LU	0.84	0/828	1.01	0/1107
42	LV	0.85	0/863	1.10	0/1156
43	LW	0.78	0/744	1.03	0/994
44	LX	0.93	0/725	1.15	0/961
45	LY	0.88	0/765	1.12	0/1025
46	La	0.84	0/602	1.13	0/797
47	Lb	0.85	0/634	1.13	0/848
48	Lc	0.66	0/502	0.95	0/667
49	Ld	0.85	0/452	1.15	0/605
50	Le	0.95	0/539	1.18	0/721
51	Lf	0.88	0/450	1.17	2/599 (0.3%)
52	Lg	0.65	0/416	0.88	0/554
53	Lh	0.82	0/380	1.19	1/498 (0.2%)
54	Li	0.88	0/521	1.19	0/687
55	Lj	0.88	0/303	1.10	0/397
56	EF	0.97	0/5277	1.26	4/7145 (0.1%)
57	Dt	0.42	0/1721	0.59	1/2682 (0.0%)
58	Pt	0.44	0/1625	0.65	0/2523
59	mR	0.38	0/239	0.64	0/370
60	B	1.67	0/18	1.03	0/22
All	All	0.59	1/165437 (0.0%)	0.78	20/246357 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
12	SL	0	1
33	LM	0	4
35	LO	0	4
41	LU	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
54	Li	0	1
All	All	0	11

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23	2552	OMU	O3'-P	5.75	1.62	1.56

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	LK	22	PRO	N-CA-C	7.77	120.17	110.70
28	LE	116	GLY	CA-C-O	-6.35	118.09	122.22
56	EF	302	GLY	CA-C-O	-6.31	117.87	122.23
56	EF	524	PRO	CB-CA-C	-6.27	105.69	111.40
36	LP	19	GLY	CA-C-O	-5.97	118.11	122.23
22	23	784	G	C2'-C3'-O3'	-5.95	104.78	113.70
51	Lf	5	GLN	N-CA-C	-5.90	106.12	113.38
53	Lh	7	PRO	N-CA-C	5.86	120.39	111.19
22	23	1083	U	C2'-C3'-O3'	5.78	122.37	113.70
8	SH	128	TYR	CB-CA-C	-5.50	101.34	110.14
18	SR	26	ILE	N-CA-C	-5.36	107.56	111.90
37	LQ	106	ASP	CB-CA-C	-5.31	100.75	109.99
56	EF	75	MET	N-CA-C	-5.28	105.61	111.36
22	23	265	A	C2'-C3'-O3'	-5.21	101.68	109.50
57	Dt	20	G	C2'-C3'-O3'	5.17	117.26	109.50
22	23	479	A	C2'-C3'-O3'	-5.16	101.77	109.50
25	LB	234	GLY	CA-C-O	-5.16	118.61	122.37
56	EF	566	LEU	CA-C-O	-5.13	115.30	120.84
35	LO	45	GLY	CA-C-O	-5.06	118.01	122.16
51	Lf	20	ASP	CA-CB-CG	5.02	117.62	112.60

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	LM	79	GLY	Mainchain
33	LM	80[A]	HIS	Mainchain
33	LM	80[B]	HIS	Mainchain
35	LO	77	ILE	Mainchain
35	LO	78[A]	ARG	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
35	LO	78[B]	ARG	Mainchain
41	LU	51	VAL	Peptide
54	Li	23[A]	LYS	Mainchain
12	SL	44	LYS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	16	32505	0	16376	222	0
2	SB	1770	0	1797	13	0
3	SC	1624	0	1696	15	0
4	SD	1642	0	1707	19	0
5	SE	1144	0	1185	13	0
6	SF	862	0	864	5	0
7	SG	1236	0	1288	11	0
8	SH	978	0	1031	6	0
9	SI	1021	0	1070	12	0
10	SJ	795	0	836	13	0
11	SK	876	0	887	12	0
12	SL	957	0	1017	8	0
13	SM	891	0	952	10	0
14	SN	804	0	844	12	0
15	SO	713	0	734	0	0
16	SP	649	0	666	4	0
17	SQ	648	0	691	2	0
18	SR	555	0	578	5	0
19	SS	668	0	693	11	0
20	ST	669	0	719	3	0
21	SU	589	0	629	5	0
22	23	62334	0	31371	317	0
23	5	2570	0	1301	5	0
24	LA	1026	0	1092	9	0
25	LB	2082	0	2154	12	0
26	LC	1565	0	1616	9	0
27	LD	1552	0	1619	8	0
28	LE	1410	0	1444	20	0
29	LF	1322	0	1371	14	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	LI	1110	0	1148	7	0
31	LJ	974	0	1011	12	0
32	LK	979	0	1028	15	0
33	LM	1138	0	1168	8	0
34	LN	946	0	1023	13	0
35	LO	1063	0	1141	14	0
36	LP	1074	0	1155	5	0
37	LQ	960	0	1000	4	0
38	LR	891	0	923	7	0
39	LS	916	0	962	4	0
40	LT	947	0	1019	5	0
41	LU	815	0	839	5	0
42	LV	856	0	922	4	0
43	LW	738	0	807	3	0
44	LX	721	0	770	5	0
45	LY	752	0	780	4	0
46	La	595	0	610	3	0
47	Lb	624	0	652	6	0
48	Lc	501	0	531	3	0
49	Ld	448	0	488	2	0
50	Le	529	0	527	6	0
51	Lf	444	0	458	5	0
52	Lg	409	0	440	2	0
53	Lh	377	0	418	1	0
54	Li	512	0	584	6	0
55	Lj	302	0	340	1	0
56	EF	5179	0	5141	74	0
57	Dt	1645	0	844	9	0
58	Pt	1637	0	843	18	0
59	mR	214	0	108	1	0
60	B	60	0	45	13	0
61	16	12	0	24	1	0
61	23	54	0	108	1	0
62	16	77	0	0	0	0
62	23	315	0	0	0	0
62	5	5	0	0	0	0
62	EF	1	0	0	0	0
62	LB	3	0	0	0	0
62	LQ	1	0	0	0	0
62	La	1	0	0	0	0
62	Pt	1	0	0	0	0
63	23	20	0	38	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	Le	1	0	0	0	0
64	Lj	1	0	0	0	0
65	EF	28	0	12	0	0
66	Pt	10	0	10	0	0
67	Pt	10	0	6	1	0
All	All	154353	0	106151	965	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 4.

All (965) 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)
60:B:7:DHA:HB2	60:B:8:SAR:HN1	1.34	1.10
67:Pt:3002:PHE:CE1	67:Pt:3002:PHE:CE2	2.41	0.99
1:16:1422:G:H5"	34:LN:48:PRO:HB3	1.47	0.95
58:Pt:64:A:C5	58:Pt:64:A:N3	2.44	0.84
56:EF:639:ARG:HD2	56:EF:691:PRO:HG2	1.67	0.75
56:EF:352:SER:HB3	56:EF:405:ILE:HG12	1.68	0.74
1:16:664:G:H22	1:16:741:G:H1	1.37	0.72
22:23:2134:A:H1'	22:23:2159:G:H1'	1.69	0.72
22:23:2443:C:O2'	22:23:2444:G:H5'	1.89	0.72
1:16:963:G:H21	10:SJ:57:VAL:HG11	1.55	0.71
22:23:2305:U:H5"	28:LE:131:GLY:HA3	1.72	0.70
1:16:202:G:H21	1:16:466:A:H61	1.38	0.70
22:23:1716:U:H2'	22:23:1717:A:C8	2.26	0.70
56:EF:417:SER:OG	60:B:4:0UO:H11	1.92	0.69
22:23:568:U:H1'	22:23:2030:6MZ:H9C1	1.74	0.69
56:EF:493:THR:HB	56:EF:613:LEU:HD11	1.74	0.69
22:23:2127:G:H2'	22:23:2128:G:C8	2.29	0.68
13:SM:85:CYS:HA	19:SS:74:PHE:HA	1.75	0.68
22:23:856:G:H2'	22:23:857:G:C8	2.29	0.68
22:23:2127:G:H2'	22:23:2128:G:H8	1.59	0.67
10:SJ:42:LEU:HB2	10:SJ:71:LEU:HB2	1.75	0.67
56:EF:404:ILE:HD11	56:EF:406:LEU:HD21	1.76	0.67
57:Dt:9:G:H5'	57:Dt:47:G7M:H1'	1.76	0.67
56:EF:10:TYR:HB3	56:EF:83:ARG:HB2	1.77	0.67
22:23:1716:U:H2'	22:23:1717:A:H8	1.60	0.67
58:Pt:15:G:H2'	58:Pt:16:H2U:H62	1.76	0.67
22:23:1792:G:H5'	25:LB:204:VAL:HG13	1.77	0.66
58:Pt:64:A:N3	58:Pt:64:A:N9	2.44	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:Pt:43:C:H2'	58:Pt:44:G:C8	2.32	0.64
1:16:1086:U:H3	1:16:1099:G:H22	1.46	0.63
1:16:352:C:H5'	61:16:1601:PUT:H21	1.79	0.63
56:EF:445:PHE:HE1	56:EF:458:ILE:HB	1.63	0.63
22:23:414:C:H2'	22:23:415:A:C8	2.34	0.63
50:Le:66:ILE:HG13	50:Le:66:ILE:O	1.98	0.62
1:16:1063:C:H2'	1:16:1064:G:C8	2.35	0.62
56:EF:317:PHE:HA	56:EF:341:GLY:HA3	1.81	0.62
22:23:1082:U:H5'	32:LK:119:GLY:HA2	1.80	0.62
29:LF:24:ILE:HG12	29:LF:72:LEU:HD21	1.82	0.62
1:16:330:C:H2'	1:16:331:G:H8	1.63	0.61
22:23:2233:U:H2'	22:23:2234:G:C8	2.35	0.61
2:SB:100:MET:HA	2:SB:107:VAL:HG21	1.81	0.61
3:SC:10:ILE:HG23	3:SC:11:ARG:HG3	1.82	0.61
11:SK:87:LYS:HG3	11:SK:115:PRO:HD3	1.80	0.61
35:LO:110:VAL:HB	35:LO:127:VAL:HG13	1.82	0.61
28:LE:132:VAL:HB	28:LE:152:LEU:HG	1.82	0.61
22:23:2122:U:H2'	22:23:2123:G:C8	2.34	0.61
28:LE:8:TYR:HB2	28:LE:173:PHE:HE1	1.64	0.61
22:23:785:G:H4'	22:23:1779:U:H4'	1.82	0.61
63:23:3011:SPD:H71	42:LV:87:PRO:HD2	1.82	0.61
56:EF:227:ALA:HB1	56:EF:234:MET:HA	1.81	0.61
1:16:350:G:H2'	1:16:351:G:C8	2.36	0.61
31:LJ:76:PHE:HA	31:LJ:80:THR:HG21	1.81	0.60
1:16:662:U:H2'	1:16:663:A:C8	2.37	0.60
22:23:2123:G:H2'	22:23:2124:G:C8	2.36	0.60
1:16:269:C:H2'	1:16:270:A:C8	2.35	0.60
22:23:1802:A:H2'	22:23:1803:A:C8	2.36	0.60
5:SE:81:LEU:HD22	5:SE:147:MET:HE1	1.83	0.60
22:23:1386:C:H2'	22:23:1387:A:C8	2.36	0.60
35:LO:58:TYR:O	54:Li:13:ARG:HD2	2.02	0.60
3:SC:70:THR:HG21	3:SC:76:VAL:HG11	1.84	0.59
4:SD:13:ARG:HD2	4:SD:32:CYS:SG	2.42	0.59
5:SE:45:ARG:HG2	5:SE:71:MET:HE2	1.83	0.59
4:SD:106:GLY:HA3	4:SD:162:ALA:HB2	1.84	0.59
1:16:946:A:H2'	1:16:947:G:C8	2.37	0.59
19:SS:9:PRO:HD3	50:Le:64:PHE:HB3	1.84	0.59
22:23:2331:G:H4'	46:La:43:THR:H	1.67	0.59
43:LW:58:VAL:HG22	43:LW:85:VAL:HG13	1.83	0.59
1:16:1162:C:H2'	1:16:1163:A:C8	2.37	0.59
1:16:477:C:H2'	1:16:478:A:C8	2.37	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:SI:84:THR:HG21	9:SI:104:VAL:HA	1.85	0.59
46:La:59:LEU:HD12	46:La:80:ILE:HD12	1.83	0.59
22:23:832:U:H2'	22:23:833:A:C8	2.38	0.58
50:Le:13:THR:HG22	50:Le:23:LYS:HG2	1.85	0.58
56:EF:94:ASP:HB3	56:EF:465:HIS:HB2	1.84	0.58
22:23:1028:A:H2'	22:23:1029:A:C8	2.38	0.58
22:23:2273:A:H2'	22:23:2274:A:C8	2.39	0.58
1:16:553:A:H5"	12:SL:21:VAL:HG21	1.85	0.58
1:16:796:C:H4'	11:SK:127:ARG:HH21	1.68	0.58
1:16:1071:C:H2'	1:16:1072:G:H8	1.69	0.58
35:LO:79:LEU:HD11	35:LO:112:LEU:HD12	1.84	0.58
1:16:713:G:H2'	1:16:714:G:C8	2.38	0.58
22:23:2636:C:H2'	22:23:2637:U:C6	2.38	0.58
56:EF:169:LEU:HD11	56:EF:263:LEU:HD13	1.86	0.58
58:Pt:23:A:H2'	58:Pt:24:G:C8	2.38	0.58
1:16:1476:A:H2'	1:16:1477:U:C6	2.39	0.58
17:SQ:9:GLN:HG2	17:SQ:60:GLU:HG2	1.86	0.57
22:23:910:A:H2'	22:23:911:A:C8	2.39	0.57
22:23:2291:U:H2'	22:23:2292:U:C6	2.39	0.57
1:16:769:G:H4'	1:16:1513:A:H4'	1.86	0.57
1:16:1097:C:H2'	1:16:1098:C:C6	2.38	0.57
22:23:2756:U:H1'	22:23:2757:A:H5"	1.86	0.57
28:LE:108:VAL:HG11	28:LE:176:PRO:HG3	1.85	0.57
56:EF:447:VAL:HG13	56:EF:458:ILE:HG22	1.87	0.57
22:23:1000:A:H2'	22:23:1001:A:C8	2.39	0.57
22:23:2314:A:H1'	28:LE:155:THR:HG21	1.85	0.57
30:LI:30:LEU:HB3	30:LI:36:ALA:HB3	1.87	0.57
35:LO:77:ILE:HD11	35:LO:110:VAL:HG22	1.85	0.57
10:SJ:12:ALA:HB3	10:SJ:18:ILE:HB	1.86	0.57
12:SL:6:GLN:HG2	12:SL:9:ARG:HH21	1.69	0.57
12:SL:50:ARG:HB3	12:SL:66:TYR:HE1	1.70	0.56
22:23:657:U:H2'	22:23:658:U:C6	2.40	0.56
1:16:1412:C:H2'	1:16:1413:A:C8	2.41	0.56
1:16:59:A:H5"	1:16:387:U:H5"	1.87	0.56
1:16:299:G:H2'	1:16:300:A:C8	2.40	0.56
22:23:373:U:H2'	22:23:374:A:H8	1.70	0.56
1:16:1347:G:H1'	1:16:1348:U:H5	1.71	0.56
20:ST:31:PHE:HB3	20:ST:54:MET:HB3	1.87	0.56
22:23:1028:A:N6	22:23:1125:G:H2'	2.20	0.56
1:16:991:U:H1'	1:16:993:G:H8	1.71	0.56
4:SD:139:PRO:HA	4:SD:182:PHE:HD2	1.71	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:Lf:12:LYS:HD3	51:Lf:15:MET:HE3	1.87	0.56
1:16:235:C:H2'	1:16:236:A:C8	2.41	0.56
1:16:492:C:H2'	1:16:493:A:C8	2.40	0.56
1:16:1356:G:H2'	1:16:1357:A:C8	2.41	0.56
30:LI:4:ILE:HD11	30:LI:44:ILE:HG12	1.87	0.56
1:16:1040:U:H2'	1:16:1041:G:C8	2.42	0.55
22:23:1429:G:H2'	22:23:1430:G:C8	2.41	0.55
33:LM:28:LEU:HD12	33:LM:142:ILE:HD13	1.88	0.55
1:16:429:U:H3'	4:SD:9:LEU:HD12	1.88	0.55
22:23:404:A:H4'	22:23:405:U:H5"	1.88	0.55
30:LI:4:ILE:HG12	30:LI:18:GLN:HG2	1.88	0.55
35:LO:57:LEU:HD22	54:Li:54:ASP:HB3	1.89	0.55
56:EF:282:VAL:O	56:EF:286:LEU:HB2	2.06	0.55
22:23:2066:C:O2'	22:23:2067:G:H5'	2.07	0.55
22:23:2788:C:H2'	22:23:2789:C:C6	2.41	0.55
1:16:473:U:H2'	1:16:474:G:C8	2.41	0.55
1:16:1038:C:H2'	1:16:1039:G:C8	2.41	0.55
22:23:2834:G:H2'	22:23:2879:A:H61	1.70	0.55
32:LK:80:LEU:HD11	32:LK:129:ILE:HG23	1.88	0.55
1:16:632:U:H4'	1:16:633:G:H8	1.72	0.55
36:LP:64:TRP:HB2	36:LP:104:GLU:HB2	1.87	0.55
1:16:427:U:H2'	1:16:428:G:C8	2.40	0.55
1:16:486:U:H2'	1:16:487:A:H8	1.71	0.55
1:16:683:G:H21	11:SK:40:ASN:HD22	1.54	0.55
1:16:744:C:H2'	1:16:745:G:H8	1.72	0.55
11:SK:52:PHE:HD2	11:SK:56:ARG:HB3	1.72	0.55
22:23:2202:U:H5"	22:23:2203:U:H5	1.71	0.55
1:16:35:G:H2'	1:16:36:C:C6	2.41	0.55
1:16:1175:G:H2'	1:16:1176:A:C8	2.42	0.55
12:SL:114:ARG:HB3	12:SL:119:VAL:HB	1.88	0.55
22:23:851:C:H2'	22:23:852:U:C6	2.42	0.55
56:EF:245:GLU:HA	56:EF:248:ILE:HG12	1.88	0.55
1:16:215:C:H2'	1:16:216:U:C6	2.41	0.54
22:23:1693:U:H5"	22:23:1694:C:H5	1.72	0.54
28:LE:58:ALA:HB2	28:LE:65:PRO:HD3	1.89	0.54
29:LF:17:VAL:HG11	29:LF:50:LEU:HD21	1.88	0.54
29:LF:37:LEU:HD12	29:LF:43:VAL:HG21	1.89	0.54
1:16:998:C:H42	1:16:1042:A:H61	1.55	0.54
22:23:2192:U:H2'	22:23:2193:G:C8	2.42	0.54
22:23:2153:C:H2'	22:23:2154:A:C8	2.42	0.54
22:23:2809:A:H2'	22:23:2810:A:C8	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:LK:97:LYS:HD3	32:LK:139:VAL:HG21	1.89	0.54
1:16:1251:A:H2'	1:16:1252:A:C8	2.42	0.54
22:23:27:G:N2	22:23:512:G:H1'	2.22	0.54
22:23:580:U:H2'	22:23:581:C:C6	2.43	0.54
22:23:2112:G:H1	22:23:2168:G:H22	1.56	0.54
1:16:1391:U:H2'	1:16:1392:G:C8	2.41	0.54
1:16:715:A:H2'	1:16:716:A:C8	2.43	0.54
22:23:2182:U:H2'	22:23:2183:A:C8	2.42	0.54
47:Lb:49:LEU:HD21	47:Lb:78:TYR:HB2	1.89	0.54
22:23:577:G:H2'	22:23:578:G:C8	2.42	0.54
56:EF:638:ARG:C	56:EF:640:GLY:H	2.16	0.54
38:LR:74:VAL:HG13	38:LR:106:LEU:HD13	1.89	0.54
58:Pt:4:C:H2'	58:Pt:5:G:C8	2.42	0.54
4:SD:101:VAL:HG12	4:SD:105:MET:HE1	1.90	0.54
4:SD:106:GLY:HA2	4:SD:165:ARG:HH21	1.73	0.54
22:23:2102:G:H1	22:23:2187:U:H3	1.56	0.54
33:LM:28:LEU:HD12	33:LM:142:ILE:CD1	2.38	0.54
1:16:67:C:H2'	1:16:68:G:C8	2.43	0.53
22:23:558:U:H2'	22:23:559:G:C8	2.43	0.53
28:LE:33:LYS:HB3	28:LE:92:ARG:HG2	1.90	0.53
27:LD:148:ILE:HB	27:LD:169:VAL:HG22	1.90	0.53
1:16:1009:U:H2'	1:16:1010:U:C6	2.44	0.53
3:SC:71:ALA:HA	3:SC:106:VAL:HB	1.90	0.53
22:23:2014:A:H2'	22:23:2015:A:C8	2.44	0.53
4:SD:9:LEU:HD13	4:SD:32:CYS:HB2	1.90	0.53
22:23:764:A:H5"	25:LB:209:GLY:CA	2.39	0.53
1:16:1308:U:H2'	1:16:1309:G:C8	2.43	0.53
19:SS:11:ILE:HD12	19:SS:38:SER:HB3	1.90	0.53
22:23:833:A:H2'	22:23:834:G:C8	2.44	0.53
22:23:1853:A:H2'	22:23:1854:A:C8	2.44	0.53
22:23:163:C:H2'	22:23:164:C:C6	2.44	0.53
8:SH:83:LEU:HD13	12:SL:4:VAL:HG11	1.91	0.53
33:LM:7:LYS:HB2	33:LM:10:THR:HG23	1.90	0.53
33:LM:17:VAL:HG23	33:LM:137:PRO:HB2	1.91	0.53
9:SI:15:SER:HB3	9:SI:70:GLY:HA3	1.92	0.52
22:23:593:U:H2'	22:23:594:U:C6	2.44	0.52
22:23:2134:A:H2'	22:23:2135:A:C8	2.44	0.52
22:23:2327:A:H2'	22:23:2328:A:C8	2.44	0.52
30:LI:48:GLU:O	30:LI:51:ARG:HG2	2.09	0.52
25:LB:21:ASN:HB3	25:LB:24:LEU:HG	1.91	0.52
49:Ld:6:LYS:HG2	49:Ld:37:GLU:HG3	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:16:997:U:H3	1:16:1043:G:H1	1.58	0.52
56:EF:38:HIS:O	56:EF:39:LYS:C	2.51	0.52
22:23:608:A:H2'	22:23:609:A:C8	2.44	0.52
22:23:1469:A:H2'	22:23:1470:A:C8	2.44	0.52
22:23:1809:A:H2'	22:23:1810:A:C8	2.44	0.52
22:23:2185:U:H2'	22:23:2186:G:C8	2.45	0.52
19:SS:53:ASN:O	19:SS:54:GLY:C	2.52	0.52
1:16:96:U:H2'	1:16:97:G:C8	2.45	0.52
24:LA:51:ASP:C	24:LA:53:ARG:H	2.16	0.52
56:EF:682:MET:HE2	60:B:3:TRP:CD2	2.45	0.52
57:Dt:62:C:H2'	57:Dt:63:C:C6	2.45	0.52
1:16:202:G:H2'	1:16:203:G:C8	2.45	0.52
1:16:458:U:H2'	1:16:459:A:C8	2.45	0.52
22:23:740:C:H5'	22:23:1784:A:H3'	1.92	0.52
22:23:1405:U:H2'	22:23:1406:U:C6	2.45	0.52
1:16:56:U:H2'	1:16:57:G:C8	2.44	0.52
22:23:812:C:H5	35:LO:21:ARG:HB3	1.74	0.52
1:16:1308:U:H2'	1:16:1309:G:H8	1.75	0.52
4:SD:104:ARG:HB3	4:SD:168:PRO:HG2	1.93	0.51
19:SS:36:ARG:HG2	19:SS:51:VAL:HG23	1.92	0.51
22:23:2328:A:H2'	22:23:2329:U:C6	2.45	0.51
22:23:881:G:H22	22:23:895:U:H3	1.58	0.51
1:16:1527:U:H5	21:SU:42:THR:HG21	1.75	0.51
22:23:1199:U:H1'	40:LT:4:VAL:HG22	1.92	0.51
28:LE:160:ALA:HB1	28:LE:165:GLU:HB2	1.92	0.51
29:LF:24:ILE:HG21	29:LF:72:LEU:HD11	1.93	0.51
1:16:204:G:H2'	1:16:205:A:C8	2.46	0.51
1:16:621:A:H2'	1:16:622:A:C8	2.45	0.51
22:23:1859:U:H2'	22:23:1860:G:C8	2.45	0.51
51:Lf:54:VAL:HG23	51:Lf:55:ILE:HG12	1.93	0.51
1:16:1071:C:H2'	1:16:1072:G:C8	2.45	0.51
1:16:1288:A:N1	1:16:1371:G:H1'	2.26	0.51
1:16:1422:G:C5'	34:LN:48:PRO:HB3	2.31	0.51
56:EF:31:LEU:HD22	56:EF:368:ALA:HB2	1.92	0.51
56:EF:536:PHE:HD1	56:EF:576:ILE:HD11	1.75	0.51
1:16:1236:A:H4'	1:16:1304:G:H4'	1.93	0.51
22:23:1923:U:H2'	22:23:1924:C:C6	2.46	0.51
30:LI:69:ALA:HB2	30:LI:138:VAL:HG11	1.92	0.51
1:16:999:C:H2'	1:16:1000:A:C8	2.46	0.51
1:16:1314:C:H2'	1:16:1315:U:C6	2.45	0.51
22:23:764:A:H5"	25:LB:209:GLY:HA2	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:SD:15:GLU:HG2	4:SD:60:LYS:HB2	1.93	0.51
1:16:407:U:H2'	1:16:408:A:C8	2.46	0.51
1:16:1001:C:H2'	1:16:1002:G:C8	2.46	0.51
8:SH:29:SER:HB2	8:SH:59:LEU:HB2	1.92	0.51
22:23:1081:U:H2'	22:23:1082:U:C6	2.46	0.51
22:23:2618:G:H21	26:LC:155:VAL:HG21	1.75	0.51
1:16:1147:C:H2'	1:16:1148:U:C6	2.46	0.51
7:SG:88:PRO:HD3	7:SG:148:ASN:HB3	1.93	0.51
11:SK:29:ASN:HB2	11:SK:57:LYS:HE2	1.92	0.51
22:23:720:U:H2'	22:23:721:A:C8	2.46	0.51
22:23:1796:U:H2'	22:23:1797:G:H8	1.76	0.51
22:23:2165:C:H42	22:23:2171:A:H62	1.59	0.51
22:23:2515:C:H2'	22:23:2516:A:C8	2.46	0.51
38:LR:75:GLY:HA2	38:LR:106:LEU:HD12	1.93	0.51
1:16:536:C:H2'	1:16:537:G:C8	2.46	0.50
22:23:396:G:H1'	47:Lb:29:PHE:HB3	1.92	0.50
22:23:1796:U:H2'	22:23:1797:G:C8	2.46	0.50
22:23:2898:U:H2'	22:23:2899:A:C8	2.46	0.50
57:Dt:24:C:H2'	57:Dt:25:U:C6	2.46	0.50
58:Pt:68:C:H2'	58:Pt:69:G:C8	2.46	0.50
1:16:993:G:H21	1:16:996:A:H61	1.58	0.50
22:23:2080:A:H5'	47:Lb:19:SER:HB2	1.93	0.50
31:LJ:48:ALA:HB3	31:LJ:95:LEU:HD11	1.93	0.50
56:EF:255:ARG:HB3	56:EF:261:ILE:HG12	1.93	0.50
1:16:40:C:H2'	1:16:41:G:C8	2.47	0.50
1:16:518:C:H2'	1:16:530:G:C8	2.47	0.50
36:LP:33:LEU:HD13	36:LP:117:PHE:HB3	1.92	0.50
1:16:536:C:H2'	1:16:537:G:H8	1.77	0.50
1:16:997:U:H2'	1:16:998:C:C6	2.47	0.50
22:23:191:A:H2'	22:23:192:C:C6	2.47	0.50
22:23:2039:U:H2'	22:23:2040:G:C8	2.46	0.50
22:23:2698:U:H2'	22:23:2699:C:C6	2.46	0.50
25:LB:77:VAL:HG22	25:LB:115:GLN:HG2	1.93	0.50
56:EF:489:ALA:HB3	60:B:8:SAR:HA3	1.93	0.50
1:16:501:C:H2'	1:16:502:A:C8	2.47	0.50
1:16:1198:G:H2'	1:16:1199:U:C6	2.47	0.50
22:23:2101:A:H2'	22:23:2102:G:C8	2.46	0.50
22:23:558:U:H2'	22:23:559:G:H8	1.76	0.50
41:LU:41:ILE:HG13	41:LU:54:VAL:HG21	1.94	0.50
43:LW:53:VAL:HG21	43:LW:87:LEU:HD21	1.94	0.50
1:16:1350:A:H2	7:SG:34:GLY:HA3	1.77	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:SG:129:GLU:HB3	7:SG:131:LYS:HD3	1.94	0.50
14:SN:62:ASN:HB3	14:SN:73:PHE:CD1	2.46	0.50
22:23:250:G:H2'	22:23:251:A:C8	2.47	0.50
22:23:1264:A:H5'	51:Lf:8:PRO:HG2	1.93	0.50
5:SE:85:VAL:HG12	5:SE:96:MET:HE3	1.94	0.50
9:SI:55:VAL:HG13	9:SI:94:LEU:HD13	1.94	0.50
22:23:2684:U:H4'	34:LN:76:VAL:CG2	2.42	0.50
4:SD:122:ALA:HB1	4:SD:149:ALA:HB2	1.93	0.50
22:23:2122:U:H2'	22:23:2123:G:H8	1.77	0.50
32:LK:97:LYS:HD3	32:LK:139:VAL:CG2	2.42	0.50
56:EF:466:LEU:O	56:EF:469:ILE:HG13	2.12	0.50
1:16:9:G:H5'	5:SE:108:GLY:HA3	1.94	0.49
1:16:1232:U:H5"	9:SI:126:GLN:HB3	1.93	0.49
24:LA:69:THR:HA	24:LA:176:GLY:HA2	1.95	0.49
58:Pt:7:A:H5"	58:Pt:8:4SU:H5	1.93	0.49
1:16:590:U:H2'	1:16:591:U:C6	2.47	0.49
1:16:744:C:H2'	1:16:745:G:C8	2.47	0.49
1:16:1225:A:H2'	1:16:1226:C:C6	2.46	0.49
7:SG:71:PRO:HD3	7:SG:100:ALA:HB2	1.92	0.49
10:SJ:80:THR:HB	10:SJ:83:THR:HG23	1.93	0.49
22:23:634:C:H2'	22:23:635:C:C6	2.48	0.49
22:23:959:A:H2'	22:23:960:A:C8	2.47	0.49
22:23:2123:G:H2'	22:23:2124:G:H8	1.76	0.49
36:LP:38:ARG:HB3	36:LP:98:PRO:HD3	1.93	0.49
56:EF:445:PHE:CE1	56:EF:458:ILE:HB	2.45	0.49
1:16:1181:G:H4'	1:16:1182:G:H5'	1.93	0.49
6:SF:101:PRO:HA	6:SF:104:LYS:HE2	1.95	0.49
23:5:5:U:H2'	23:5:6:G:C8	2.48	0.49
56:EF:174:GLY:HA3	56:EF:179:PHE:HA	1.93	0.49
22:23:2554:U:H2'	22:23:2555:U:C6	2.47	0.49
40:LT:49:ASP:HA	40:LT:52:GLN:HB2	1.95	0.49
42:LV:24:ILE:HD13	42:LV:36:LEU:HD11	1.94	0.49
50:Le:5:ILE:HG13	50:Le:6:HIS:HD2	1.77	0.49
1:16:1048:G:H2'	1:16:1050:G:C8	2.48	0.49
22:23:1040:A:H2	22:23:1115:G:H22	1.59	0.49
22:23:1432:G:H2'	22:23:1433:A:C8	2.47	0.49
56:EF:465:HIS:O	56:EF:468:ILE:HG13	2.12	0.49
16:SP:4:ILE:HG12	16:SP:21:VAL:HG22	1.94	0.49
22:23:465:G:H2'	22:23:466:A:C8	2.47	0.49
1:16:514:C:H2'	1:16:515:G:C8	2.48	0.49
2:SB:24:ASN:HD22	2:SB:27:MET:HG2	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:23:1495:A:H2'	22:23:1496:A:C8	2.48	0.49
1:16:310:G:H5"	16:SP:31:ARG:HB3	1.94	0.49
1:16:1338:G:H2'	1:16:1339:A:C8	2.47	0.49
1:16:1384:C:H2'	1:16:1385:G:C8	2.47	0.49
1:16:1391:U:H2'	1:16:1392:G:H8	1.78	0.49
3:SC:64:ILE:HG13	3:SC:99:ALA:HA	1.94	0.49
6:SF:7:VAL:HG22	6:SF:61:LEU:HD13	1.95	0.49
28:LE:62:GLY:O	50:Le:7:PRO:HD2	2.13	0.49
28:LE:103:LEU:HD12	28:LE:107:ALA:HB3	1.95	0.49
35:LO:63:LYS:HA	54:Li:13:ARG:HG3	1.95	0.49
1:16:1:A:H2'	1:16:1:A:N3	2.28	0.48
1:16:1021:A:H2'	1:16:1022:A:C8	2.48	0.48
5:SE:34:THR:HG22	5:SE:52:LYS:HG2	1.95	0.48
22:23:244:A:H5"	35:LO:67:THR:HG21	1.95	0.48
22:23:1438:U:H2'	22:23:1439:A:H8	1.78	0.48
22:23:2074:U:H2'	22:23:2075:U:C6	2.48	0.48
29:LF:33:LEU:HD11	29:LF:136:ALA:O	2.13	0.48
56:EF:282:VAL:HA	56:EF:286:LEU:HD13	1.95	0.48
58:Pt:9:A:H5"	58:Pt:46:G7M:H1'	1.94	0.48
1:16:893:C:H2'	1:16:894:G:C8	2.48	0.48
11:SK:45:ALA:HB3	11:SK:70:CYS:HB2	1.95	0.48
22:23:1309:G:H4'	53:Lh:7:PRO:HB2	1.95	0.48
44:LX:12:ILE:HD11	44:LX:20:GLY:HA2	1.94	0.48
2:SB:57:LEU:HD13	2:SB:217:VAL:HG13	1.93	0.48
22:23:1056:G:H4'	22:23:1086:A:C8	2.48	0.48
22:23:1056:G:H4'	22:23:1086:A:H8	1.77	0.48
56:EF:288:SER:HB3	56:EF:289:PRO:HD2	1.95	0.48
1:16:1369:C:H2'	1:16:1370:G:C8	2.47	0.48
22:23:284:U:H2'	22:23:285:G:C8	2.49	0.48
32:LK:14:ALA:HA	32:LK:54:PRO:HA	1.96	0.48
45:LY:72:VAL:HG12	45:LY:93:ARG:HA	1.95	0.48
1:16:1414:U:H2'	1:16:1415:G:H8	1.77	0.48
3:SC:129:MET:HE3	3:SC:132:ARG:HB2	1.95	0.48
22:23:2099:U:H2'	22:23:2100:G:C8	2.49	0.48
56:EF:282:VAL:HG13	56:EF:286:LEU:HD22	1.94	0.48
1:16:1329:A:H5"	13:SM:26:GLY:H	1.78	0.48
9:SI:120:LYS:HB2	9:SI:123:ARG:HB3	1.95	0.48
11:SK:31:ILE:HG12	11:SK:46:THR:HG22	1.96	0.48
16:SP:6:LEU:HB3	16:SP:17:TYR:HB3	1.95	0.48
22:23:1057:A:H1'	31:LJ:35:VAL:HG11	1.95	0.48
22:23:1231:U:H2'	22:23:1232:G:H8	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:EF:388:LEU:HD13	56:EF:391:VAL:HG21	1.95	0.48
56:EF:396:THR:HG21	56:EF:406:LEU:H	1.78	0.48
1:16:958:A:N1	19:SS:54:GLY:HA3	2.28	0.48
22:23:1544:A:H2'	22:23:1545:A:C8	2.48	0.48
28:LE:8:TYR:HB2	28:LE:173:PHE:CE1	2.48	0.48
28:LE:10:ASP:O	28:LE:14:LYS:NZ	2.33	0.48
41:LU:63:VAL:HA	41:LU:96:VAL:HG12	1.96	0.48
52:Lg:33:LYS:HD3	52:Lg:51:GLU:HB3	1.94	0.48
1:16:1011:C:H2'	1:16:1012:A:C8	2.48	0.48
3:SC:64:ILE:HG12	3:SC:97:VAL:HG23	1.95	0.48
19:SS:52:HIS:HA	19:SS:57:HIS:HA	1.95	0.48
57:Dt:33:OMC:HM22	57:Dt:34:U:H5'	1.96	0.48
1:16:466:A:H1'	1:16:467:U:H2'	1.95	0.48
1:16:613:C:H2'	1:16:614:C:C6	2.49	0.48
22:23:29:U:H2'	22:23:30:G:C8	2.49	0.48
22:23:158:U:H2'	22:23:159:G:C8	2.49	0.48
22:23:871:U:H2'	22:23:872:U:C6	2.49	0.48
1:16:1404:C:H2'	1:16:1405:G:C8	2.49	0.48
22:23:1794:A:H2'	22:23:1795:C:C6	2.49	0.48
56:EF:366:MET:HE2	56:EF:371:ARG:HD2	1.95	0.48
56:EF:643:LYS:HD2	56:EF:643:LYS:HA	1.63	0.48
3:SC:42:TYR:HD1	3:SC:45:LYS:HE2	1.78	0.47
23:5:5:U:H2'	23:5:6:G:H8	1.79	0.47
35:LO:121:THR:HA	35:LO:141:LYS:O	2.14	0.47
56:EF:268:SER:OG	56:EF:271:LYS:HB2	2.14	0.47
57:Dt:48:U:H1'	57:Dt:49:C:C5	2.49	0.47
47:Lb:5:CYS:HB2	47:Lb:33:LEU:HD11	1.96	0.47
1:16:337:G:H2'	1:16:338:A:C8	2.50	0.47
22:23:832:U:H2'	22:23:833:A:H8	1.78	0.47
22:23:2515:C:H2'	22:23:2516:A:H8	1.79	0.47
23:5:40:U:H1'	23:5:45:A:H61	1.79	0.47
1:16:216:U:H2'	1:16:217:C:C6	2.49	0.47
1:16:673:A:H2'	1:16:674:G:C8	2.49	0.47
12:SL:110:ARG:HB3	12:SL:119:VAL:HG21	1.95	0.47
22:23:980:A:H2'	22:23:981:A:C8	2.49	0.47
22:23:2243:U:H2'	22:23:2244:U:C6	2.50	0.47
22:23:2660:A:H4'	56:EF:121:PRO:HG2	1.96	0.47
22:23:796:C:H2'	22:23:797:G:C8	2.50	0.47
22:23:1170:C:H2'	22:23:1171:G:C8	2.50	0.47
24:LA:16:ASP:O	24:LA:21:TYR:OH	2.30	0.47
31:LJ:31:ARG:HB2	31:LJ:79:PRO:HG2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:EF:104:ARG:HD3	56:EF:409:MET:HG2	1.96	0.47
4:SD:101:VAL:HG12	4:SD:105:MET:CE	2.45	0.47
57:Dt:62:C:H2'	57:Dt:63:C:H6	1.79	0.47
1:16:846:G:H2'	1:16:847:G:C8	2.50	0.47
1:16:978:A:N6	1:16:1316:G:H1'	2.30	0.47
1:16:1436:U:H2'	1:16:1437:A:C8	2.49	0.47
2:SB:130:THR:C	2:SB:132:LYS:H	2.22	0.47
3:SC:22:TRP:HB3	3:SC:59:ARG:H	1.80	0.47
10:SJ:41:PRO:HA	10:SJ:72:ARG:HD3	1.97	0.47
14:SN:51:LEU:HB3	14:SN:52:PRO:HD2	1.97	0.47
22:23:414:C:H2'	22:23:415:A:H8	1.79	0.47
22:23:764:A:H2	25:LB:218:PRO:HG3	1.79	0.47
22:23:1321:A:H2'	22:23:1322:A:C8	2.49	0.47
22:23:1655:A:C2	22:23:2049:G:H5"	2.49	0.47
22:23:2016:U:H2'	22:23:2017:U:C6	2.50	0.47
22:23:2100:G:H2'	22:23:2101:A:C8	2.50	0.47
56:EF:34:THR:HG22	56:EF:72:TRP:HB2	1.97	0.47
22:23:848:C:H2'	22:23:849:A:C8	2.50	0.47
34:LN:41:ILE:HG13	34:LN:58:LEU:O	2.15	0.47
22:23:661:A:H4'	35:LO:13:LYS:HE3	1.97	0.47
22:23:1079:C:H2'	22:23:1080:A:C8	2.50	0.47
22:23:1744:A:H3'	22:23:1745:A:H8	1.79	0.47
22:23:2241:A:H2'	22:23:2242:G:C8	2.49	0.47
22:23:2313:C:H5"	28:LE:88:LYS:HD2	1.96	0.47
37:LQ:51:LEU:HB3	37:LQ:79:LEU:HD21	1.97	0.47
56:EF:136:PRO:HB3	56:EF:256:VAL:HG12	1.97	0.47
1:16:268:U:H2'	1:16:269:C:C6	2.50	0.47
22:23:948:C:H2'	22:23:949:G:H8	1.80	0.47
22:23:2566:A:N1	34:LN:28:SER:HB2	2.30	0.47
2:SB:32:PHE:HB2	2:SB:42:ASN:HB3	1.98	0.46
22:23:2812:G:H2'	22:23:2813:A:C8	2.50	0.46
58:Pt:8:4SU:H1'	58:Pt:48:C:H1'	1.98	0.46
10:SJ:4:GLN:O	10:SJ:79:PRO:HG3	2.15	0.46
22:23:1548:A:H2'	22:23:1549:A:C8	2.50	0.46
22:23:2443:C:C2'	22:23:2444:G:H5'	2.44	0.46
56:EF:155:VAL:HG13	56:EF:166:PRO:HB2	1.98	0.46
22:23:155:A:H2'	22:23:156:A:C8	2.50	0.46
22:23:321:U:H5"	27:LD:131:THR:HG23	1.97	0.46
22:23:1084:A:H2'	22:23:1085:A:C8	2.50	0.46
22:23:2398:U:H2'	22:23:2399:G:C8	2.49	0.46
58:Pt:43:C:H2'	58:Pt:44:G:H8	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:23:2107:G:H1	22:23:2182:U:H3	1.63	0.46
27:LD:147:LEU:HD12	27:LD:168:ASP:HB3	1.97	0.46
1:16:34:C:H2'	1:16:35:G:C8	2.50	0.46
1:16:486:U:H2'	1:16:487:A:C8	2.49	0.46
1:16:1039:G:H2'	1:16:1040:U:C6	2.50	0.46
11:SK:85:MET:HB3	11:SK:113:VAL:HG21	1.97	0.46
22:23:1181:U:H2'	22:23:1182:G:C8	2.50	0.46
22:23:2233:U:H2'	22:23:2234:G:H8	1.80	0.46
22:23:2419:U:H4'	52:Lg:22:THR:HG21	1.97	0.46
22:23:2804:U:H2'	22:23:2805:C:C6	2.50	0.46
41:LU:71:LYS:HA	41:LU:90:ARG:HG2	1.98	0.46
1:16:412:A:H4'	1:16:413:G:H5'	1.97	0.46
1:16:718:A:H4'	21:SU:35:ARG:HH22	1.80	0.46
14:SN:69:ARG:HB3	14:SN:80:SER:OG	2.15	0.46
22:23:1539:U:H2'	22:23:1540:G:C8	2.50	0.46
22:23:2636:C:H2'	22:23:2637:U:H6	1.78	0.46
22:23:2684:U:H4'	34:LN:76:VAL:HG21	1.96	0.46
55:Lj:1:MET:HG3	55:Lj:34:LYS:HG2	1.97	0.46
56:EF:333:LEU:HD23	56:EF:386:ILE:HG12	1.98	0.46
1:16:579:A:H2'	1:16:580:C:C6	2.50	0.46
1:16:911:U:H2'	1:16:912:C:C6	2.50	0.46
7:SG:111:ARG:HD2	7:SG:123:GLU:HG2	1.97	0.46
22:23:546:U:O2'	22:23:547:A:H5"	2.16	0.46
22:23:1357:C:H2'	22:23:1358:G:O4'	2.16	0.46
22:23:1579:A:H2'	22:23:1580:A:C8	2.50	0.46
1:16:962:C:H2'	1:16:963:G:C8	2.50	0.46
24:LA:26:ALA:HB1	24:LA:214:ILE:HD11	1.97	0.46
32:LK:80:LEU:HD21	32:LK:129:ILE:HG23	1.97	0.46
37:LQ:28:LEU:HD13	37:LQ:34:ILE:HG12	1.98	0.46
49:Ld:6:LYS:HB2	49:Ld:58:GLU:HG2	1.97	0.46
1:16:96:U:H2'	1:16:97:G:H8	1.81	0.46
1:16:1086:U:H3	1:16:1099:G:H1	1.63	0.46
22:23:627:A:H5"	35:LO:78[A]:ARG:HH21	1.81	0.46
56:EF:278:MET:HE3	56:EF:278:MET:HB3	1.83	0.46
56:EF:306:PRO:HB2	56:EF:308:GLU:HG3	1.98	0.46
1:16:839:C:H2'	1:16:840:C:C6	2.51	0.46
1:16:1035:A:H2'	1:16:1036:A:H8	1.81	0.46
1:16:1413:A:H2	1:16:1487:G:H22	1.64	0.46
22:23:492:A:H2'	22:23:493:G:O4'	2.16	0.46
22:23:2339:C:H2'	22:23:2340:A:C8	2.51	0.46
22:23:2845:U:H5"	39:LS:52:ASN:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:LF:107:LEU:HD13	29:LF:152:ARG:HB2	1.98	0.46
56:EF:517:HIS:HB3	56:EF:582:SER:HB3	1.97	0.46
1:16:95:C:H2'	1:16:96:U:C6	2.51	0.45
1:16:1079:G:H2'	1:16:1080:A:C8	2.51	0.45
4:SD:61:VAL:HG21	4:SD:200:ILE:HD11	1.98	0.45
4:SD:125:VAL:HG22	4:SD:143:VAL:HG22	1.97	0.45
22:23:1689:A:H2'	22:23:1690:A:C8	2.51	0.45
28:LE:105:THR:HA	50:Le:38:SER:HB2	1.98	0.45
1:16:266:G:N3	1:16:266:G:H2'	2.32	0.45
1:16:514:C:H2'	1:16:515:G:H8	1.81	0.45
6:SF:77:THR:O	6:SF:81:ASN:HB2	2.16	0.45
22:23:685:A:H5"	22:23:788:A:H62	1.81	0.45
22:23:1429:G:H2'	22:23:1430:G:H8	1.80	0.45
22:23:2567:G:H2'	22:23:2568:U:C6	2.52	0.45
31:LJ:54:VAL:HG22	31:LJ:81:LEU:HG	1.98	0.45
60:B:4:0UO:N	60:B:4:0UO:O3	2.49	0.45
1:16:922:G:H4'	5:SE:25:VAL:HA	1.98	0.45
1:16:1118:U:H2'	1:16:1119:C:C6	2.52	0.45
1:16:1316:G:N2	1:16:1318:A:H3'	2.32	0.45
18:SR:42:SER:HA	18:SR:45:THR:HG22	1.98	0.45
24:LA:51:ASP:C	24:LA:53:ARG:N	2.74	0.45
1:16:407:U:H5"	4:SD:112:ALA:HB1	1.98	0.45
3:SC:43:LEU:O	3:SC:47:LEU:HB2	2.17	0.45
22:23:1746:A:H2'	22:23:1747:U:C6	2.51	0.45
22:23:2598:A:H5"	25:LB:234:GLY:HA3	1.99	0.45
30:LI:132:PHE:HB2	30:LI:140:ALA:HB3	1.98	0.45
56:EF:18:HIS:ND1	56:EF:122:GLN:HB2	2.30	0.45
56:EF:103:MET:HE2	56:EF:130:ALA:HB2	1.99	0.45
1:16:714:G:H2'	1:16:715:A:C8	2.52	0.45
3:SC:20:SER:HB3	3:SC:22:TRP:NE1	2.32	0.45
3:SC:107:ARG:O	3:SC:109:PRO:HD3	2.16	0.45
22:23:1935:G:H1'	22:23:1964:G:N2	2.31	0.45
29:LF:17:VAL:HG13	29:LF:24:ILE:HD11	1.99	0.45
36:LP:20:LEU:HD13	45:LY:81:PRO:HG2	1.99	0.45
7:SG:80:VAL:H	7:SG:85:TYR:HE2	1.64	0.45
22:23:948:C:H2'	22:23:949:G:C8	2.52	0.45
42:LV:20:VAL:HG11	42:LV:44:ALA:HA	1.98	0.45
1:16:993:G:H2'	1:16:995:C:H41	1.82	0.45
12:SL:55:VAL:HG21	12:SL:80:ILE:HD11	1.99	0.45
22:23:1107:G:H4'	31:LJ:78:GLY:C	2.41	0.45
22:23:1224:U:H2'	22:23:1225:G:C8	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:23:2137:U:H2'	22:23:2138:G:C8	2.51	0.45
22:23:2251:OMG:H1'	22:23:2251:OMG:HM23	1.53	0.45
26:LC:14:ILE:HG12	26:LC:24:VAL:HG21	1.98	0.45
56:EF:473:MET:HA	56:EF:477:PHE:HD2	1.81	0.45
1:16:34:C:H2'	1:16:35:G:H8	1.82	0.45
1:16:1317:C:H4'	14:SN:48:LEU:HD21	1.99	0.45
22:23:491:G:H2'	22:23:492:A:C8	2.52	0.45
28:LE:38:MET:HE3	28:LE:38:MET:HB2	1.92	0.45
34:LN:68:GLY:HA3	34:LN:78:ARG:HG2	1.99	0.45
1:16:998:C:H2'	1:16:999:C:H6	1.82	0.45
14:SN:27:LEU:HA	14:SN:30:ILE:HG12	1.99	0.45
22:23:1102:C:H2'	22:23:1103:A:C8	2.52	0.45
26:LC:48:ILE:HG21	26:LC:90:PHE:HB2	1.99	0.45
1:16:148:G:H1'	1:16:1447:A:H1'	1.99	0.45
22:23:2086:U:H2'	22:23:2087:G:C8	2.52	0.45
22:23:2329:U:H2'	22:23:2330:G:C8	2.52	0.45
31:LJ:118:ILE:HG23	31:LJ:122:GLN:HB2	1.98	0.45
44:LX:74:ASN:C	44:LX:76:ALA:H	2.25	0.45
56:EF:67:ALA:HA	56:EF:87:ILE:HG12	1.99	0.45
56:EF:448:TRP:CD1	60:B:6:DBB:HG1	2.52	0.45
1:16:94:G:H4'	1:16:95:C:H5'	1.98	0.44
1:16:404:G:N7	4:SD:2:ALA:HB3	2.32	0.44
1:16:464:U:C2	1:16:466:A:H2'	2.51	0.44
10:SJ:46:LYS:HG2	10:SJ:68:ARG:HG2	1.99	0.44
13:SM:4:ILE:HG23	13:SM:6:GLY:H	1.82	0.44
22:23:366:C:H2'	22:23:367:G:C8	2.52	0.44
22:23:1183:U:H2'	22:23:1184:U:C6	2.52	0.44
31:LJ:111:ALA:HB3	31:LJ:118:ILE:HG22	1.99	0.44
34:LN:41:ILE:HG12	34:LN:60:ALA:HB2	1.98	0.44
44:LX:33:LYS:HB3	44:LX:64:ALA:HB1	1.99	0.44
1:16:736:C:H2'	1:16:737:C:C6	2.52	0.44
1:16:1239:A:H62	1:16:1299:A:H62	1.64	0.44
6:SF:88:MET:HB2	18:SR:65:LEU:HD21	1.99	0.44
17:SQ:46:VAL:HG21	17:SQ:61:ILE:HG21	1.98	0.44
22:23:623:C:H2'	22:23:624:C:C6	2.51	0.44
22:23:2601:C:H2'	22:23:2603:G:C8	2.51	0.44
32:LK:100:LYS:HG3	32:LK:139:VAL:HB	1.99	0.44
37:LQ:79:LEU:HD12	37:LQ:83:LEU:HD12	1.99	0.44
1:16:97:G:H3'	1:16:98:A:H8	1.81	0.44
2:SB:97:LEU:HB2	2:SB:100:MET:HE3	1.98	0.44
4:SD:105:MET:HG2	4:SD:180:GLY:HA3	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:SE:115:LEU:HD13	5:SE:123:VAL:HG11	1.98	0.44
13:SM:10:PRO:HB3	13:SM:22:ILE:HD11	1.99	0.44
22:23:721:A:H2'	22:23:722:A:C8	2.53	0.44
22:23:1102:C:H2'	22:23:1103:A:H8	1.81	0.44
22:23:1874:C:H2'	22:23:1875:G:O4'	2.18	0.44
22:23:2834:G:H2'	22:23:2879:A:N6	2.32	0.44
56:EF:280:ASP:O	56:EF:283:ILE:HG12	2.17	0.44
56:EF:444:SER:HB2	56:EF:461:MET:HG2	2.00	0.44
1:16:456:A:H2'	1:16:457:G:C8	2.52	0.44
1:16:1030:U:OP2	1:16:1031:C:N4	2.51	0.44
1:16:1323:G:H2'	1:16:1324:A:C8	2.52	0.44
22:23:373:U:H2'	22:23:374:A:C8	2.50	0.44
22:23:542:C:H2'	22:23:543:G:C8	2.52	0.44
32:LK:9:VAL:HB	32:LK:59:ILE:HG23	1.99	0.44
39:LS:9:GLU:HA	39:LS:55:LEU:HD22	1.98	0.44
1:16:407:U:H2'	1:16:408:A:H8	1.83	0.44
1:16:1130:A:H2'	1:16:1131:G:O4'	2.17	0.44
22:23:2038:G:H2'	22:23:2039:U:O4'	2.18	0.44
22:23:2289:G:H5"	22:23:2384:U:H1'	1.99	0.44
56:EF:495:ARG:HB2	56:EF:609:LYS:HB2	2.00	0.44
1:16:147:G:H2'	1:16:148:G:C8	2.53	0.44
1:16:1005:A:H2'	1:16:1006:G:O4'	2.17	0.44
22:23:2:G:H2'	22:23:3:U:C6	2.53	0.44
22:23:1908:C:O2'	58:Pt:12:U:H5"	2.18	0.44
24:LA:23:ILE:HD11	24:LA:189:LEU:HD21	1.99	0.44
32:LK:75:PRO:HG2	32:LK:78:VAL:HG22	1.98	0.44
38:LR:28:VAL:HG21	38:LR:92:PHE:CZ	2.52	0.44
48:Lc:6:LEU:HB3	48:Lc:56:LEU:HD12	2.00	0.44
1:16:1288:A:H2'	1:16:1289:A:C8	2.53	0.44
7:SG:138:ARG:HG2	7:SG:142:HIS:HD2	1.82	0.44
11:SK:113:VAL:HG13	18:SR:73:ARG:HD2	1.99	0.44
22:23:538:A:H2'	22:23:539:G:O4'	2.18	0.44
22:23:632:A:H2'	22:23:633:A:C8	2.52	0.44
22:23:2238:G:H2'	22:23:2238:G:N3	2.32	0.44
39:LS:89:ARG:HB3	39:LS:113:ARG:HB3	1.99	0.44
2:SB:114:LEU:HB2	2:SB:144:LEU:HB3	2.00	0.44
22:23:674:G:H5"	27:LD:71:GLY:N	2.32	0.44
22:23:2859:G:H2'	22:23:2860:A:C8	2.53	0.44
41:LU:6:GLN:HB3	41:LU:11:GLN:HG2	1.99	0.44
58:Pt:53:G:H2'	58:Pt:54:U:C6	2.53	0.44
1:16:62:U:H2'	1:16:63:C:C6	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:SJ:53:ILE:HG22	14:SN:85:ARG:HD2	2.00	0.44
13:SM:19:LEU:HD23	13:SM:33:ILE:HD11	1.99	0.44
18:SR:48:ARG:HB2	18:SR:51:TYR:HD2	1.82	0.44
22:23:17:G:H4'	40:LT:25:TYR:CE1	2.53	0.44
22:23:674:G:H2'	22:23:804:A:H61	1.83	0.44
22:23:830:G:H2'	61:23:3004:PUT:H31	2.00	0.44
22:23:1188:U:H2'	22:23:1189:A:H8	1.83	0.44
22:23:2731:G:H2'	22:23:2732:G:C8	2.53	0.44
31:LJ:55:VAL:HB	31:LJ:60:LEU:HG	1.99	0.44
38:LR:75:GLY:CA	38:LR:106:LEU:HD12	2.48	0.44
1:16:413:G:H1'	1:16:428:G:H21	1.83	0.43
2:SB:54:LEU:HB3	2:SB:220:THR:HG21	2.00	0.43
8:SH:76:GLN:O	8:SH:127:CYS:HB2	2.17	0.43
22:23:5:A:H2'	22:23:6:A:C8	2.53	0.43
22:23:279:A:N6	22:23:361:G:H1'	2.33	0.43
22:23:1946:U:H2'	22:23:1947:C:C6	2.53	0.43
22:23:2661:G:H4'	56:EF:19:ILE:HD13	2.00	0.43
35:LO:21:ARG:HA	35:LO:21:ARG:HD3	1.66	0.43
48:Lc:10:SER:OG	48:Lc:11:VAL:N	2.51	0.43
1:16:674:G:H2'	1:16:675:A:C8	2.52	0.43
1:16:916:U:H2'	1:16:917:G:C8	2.53	0.43
1:16:1366:C:H2'	1:16:1367:C:C6	2.54	0.43
18:SR:20:GLU:HG3	18:SR:21:ILE:H	1.83	0.43
22:23:671:C:H2'	22:23:672:C:C6	2.54	0.43
22:23:1782:U:H1'	22:23:2609:U:H5"	2.00	0.43
22:23:1853:A:N1	22:23:2087:G:H1'	2.32	0.43
22:23:2105:U:H2'	22:23:2106:U:C6	2.53	0.43
1:16:219:U:H2'	1:16:220:G:C8	2.53	0.43
1:16:868:C:H2'	1:16:869:G:O4'	2.19	0.43
1:16:1463:U:H2'	1:16:1464:U:C6	2.53	0.43
9:SI:21:ILE:HG12	9:SI:86:ALA:HB1	1.99	0.43
9:SI:21:ILE:CG1	9:SI:86:ALA:HB1	2.48	0.43
22:23:749:A:H4'	22:23:1271:G:N3	2.33	0.43
22:23:948:C:H1'	22:23:984:A:C8	2.53	0.43
22:23:1406:U:H2'	22:23:1407:G:C8	2.54	0.43
22:23:1783:A:N1	22:23:2587:A:H2'	2.33	0.43
22:23:2615:U:C2	51:Lf:4:GLN:HA	2.53	0.43
31:LJ:42:ARG:HH12	31:LJ:81:LEU:HD11	1.82	0.43
1:16:465:A:H2'	1:16:466:A:C8	2.52	0.43
1:16:819:A:H5'	1:16:820:U:H5	1.83	0.43
1:16:1517:G:C5	22:23:1920:C:H5"	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:SE:56:VAL:N	5:SE:57:PRO:HD2	2.34	0.43
22:23:284:U:H2'	22:23:285:G:H8	1.83	0.43
22:23:2619:C:H5"	26:LC:157:LYS:HA	2.00	0.43
47:Lb:7:VAL:HG21	47:Lb:59:ILE:HD11	1.99	0.43
56:EF:671:ARG:HG2	56:EF:676:GLY:HA2	2.00	0.43
1:16:490:C:H2'	1:16:491:G:C8	2.53	0.43
1:16:947:G:H4'	1:16:1332:A:H2	1.83	0.43
1:16:995:C:H2'	1:16:996:A:C8	2.53	0.43
1:16:1043:G:H2'	1:16:1044:A:C8	2.54	0.43
13:SM:58:ASP:OD1	13:SM:59:GLU:N	2.52	0.43
13:SM:106:ALA:O	13:SM:110:LYS:HG2	2.17	0.43
22:23:247:G:H4'	22:23:386:G:C5	2.53	0.43
22:23:1720:U:H2'	22:23:1721:G:O4'	2.18	0.43
22:23:2584:U:H2'	22:23:2585:U:H2'	2.01	0.43
22:23:2597:G:H5'	25:LB:241:GLY:HA3	2.01	0.43
29:LF:37:LEU:HD13	29:LF:68:ALA:HB1	2.01	0.43
60:B:7:DHA:O	60:B:8:SAR:C	2.66	0.43
1:16:490:C:H2'	1:16:491:G:H8	1.83	0.43
1:16:1206:G:H4'	3:SC:192:THR:O	2.18	0.43
1:16:1216:A:H5"	14:SN:5:SER:HB3	2.01	0.43
1:16:1517:G:H2'	1:16:1518:MA6:C8	2.49	0.43
16:SP:23:ASP:HB3	16:SP:26:ASN:ND2	2.33	0.43
22:23:52:A:H2'	22:23:53:A:C8	2.54	0.43
22:23:598:U:H2'	22:23:599:A:C8	2.53	0.43
22:23:1727:C:H2'	22:23:1728:C:C6	2.54	0.43
22:23:2186:G:H2'	22:23:2187:U:C6	2.54	0.43
25:LB:205:LEU:HB3	25:LB:210:ALA:HB3	2.01	0.43
28:LE:4:LEU:HD12	28:LE:4:LEU:HA	1.83	0.43
45:LY:6:ALA:HB2	45:LY:42:LEU:HD23	1.99	0.43
1:16:995:C:H2'	1:16:996:A:H8	1.84	0.43
1:16:1253:G:H2'	1:16:1254:A:C8	2.54	0.43
8:SH:11:LEU:HD22	8:SH:75:ILE:HD11	2.01	0.43
20:ST:78:ASN:O	20:ST:82:GLN:HG2	2.19	0.43
21:SU:58:LYS:O	21:SU:62:ARG:HG3	2.19	0.43
22:23:349:U:H2'	22:23:350:G:H8	1.83	0.43
40:LT:72:ASN:HB3	40:LT:110:VAL:HG11	2.01	0.43
56:EF:255:ARG:HG2	56:EF:260:GLU:HB2	2.01	0.43
1:16:176:C:H2'	1:16:177:G:N3	2.34	0.43
1:16:1041:G:H2'	1:16:1042:A:C8	2.54	0.43
8:SH:27:MET:HE2	8:SH:27:MET:HB3	1.94	0.43
21:SU:39:GLU:HG2	21:SU:43:THR:HB	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:23:82:U:H2'	22:23:83:A:C8	2.54	0.43
22:23:1178:C:H2'	22:23:1179:G:C8	2.53	0.43
22:23:1854:A:N6	22:23:1888:G:H1'	2.34	0.43
22:23:2547:A:H4'	34:LN:29:HIS:CE1	2.54	0.43
22:23:2845:U:H2'	22:23:2846:G:C8	2.54	0.43
26:LC:184:ARG:O	26:LC:186:LEU:HG	2.18	0.43
29:LF:105:LEU:HD21	29:LF:148:LEU:HD12	2.00	0.43
60:B:3:TRP:CH2	60:B:5:GLY:HA3	2.53	0.43
1:16:297:G:H4'	1:16:557:G:H4'	2.00	0.43
1:16:1239:A:H4'	1:16:1241:G:C8	2.54	0.43
9:SI:11:ARG:HB3	9:SI:106:ARG:HH21	1.84	0.43
22:23:739:A:H1'	22:23:740:C:H5	1.83	0.43
22:23:839:U:H2'	22:23:840:C:C6	2.54	0.43
22:23:1859:U:H2'	22:23:1860:G:H8	1.83	0.43
22:23:2099:U:H2'	22:23:2100:G:H8	1.84	0.43
37:LQ:2:ARG:HG2	37:LQ:5:LYS:HB2	2.00	0.43
44:LX:72:ILE:HD13	44:LX:103:ILE:HD13	2.01	0.43
56:EF:623:THR:HG22	56:EF:624:PRO:O	2.18	0.43
1:16:1321:U:H1'	19:SS:77:THR:HG21	2.00	0.43
2:SB:14:VAL:HG21	2:SB:213:TYR:CE2	2.53	0.43
4:SD:19:LEU:HB2	4:SD:21:LEU:HG	2.01	0.43
22:23:143:C:H2'	22:23:144:A:H8	1.84	0.43
22:23:651:G:H5'	54:Li:19:LYS:HG2	2.00	0.43
22:23:2377:A:H2'	22:23:2378:A:C8	2.54	0.43
29:LF:11:VAL:HG23	29:LF:15:VAL:HB	2.00	0.43
60:B:3:TRP:CZ3	60:B:5:GLY:HA3	2.54	0.43
1:16:235:C:H2'	1:16:236:A:H8	1.84	0.42
1:16:398:U:H2'	1:16:399:G:C8	2.53	0.42
1:16:1517:G:H2'	1:16:1518:MA6:H8	2.00	0.42
12:SL:24:LEU:HD12	12:SL:24:LEU:HA	1.83	0.42
20:ST:42:GLY:HA2	20:ST:86:LEU:HD11	2.00	0.42
22:23:594:U:H2'	22:23:595:C:C6	2.54	0.42
22:23:2016:U:H1'	51:Lf:3:VAL:HG21	2.00	0.42
38:LR:28:VAL:HG11	38:LR:103:VAL:HG13	2.01	0.42
56:EF:6:PRO:C	56:EF:8:ALA:H	2.27	0.42
10:SJ:25:ILE:HG13	10:SJ:26:VAL:N	2.34	0.42
14:SN:88:ALA:HB2	14:SN:96:LEU:HD23	2.01	0.42
22:23:166:U:H2'	22:23:167:A:C8	2.54	0.42
22:23:1425:G:H2'	22:23:1426:G:C8	2.55	0.42
22:23:1463:C:H2'	22:23:1464:G:C8	2.55	0.42
23:5:39:A:H2'	23:5:40:U:C6	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:LK:74:PRO:HG2	32:LK:79:LEU:HD21	2.01	0.42
1:16:463:U:H2'	1:16:464:U:C2	2.54	0.42
1:16:636:U:H2'	1:16:637:C:C6	2.54	0.42
1:16:1014:A:N3	1:16:1219:A:H1'	2.34	0.42
9:SI:42:GLU:HA	9:SI:45:ARG:HE	1.83	0.42
22:23:742:A:H2'	22:23:743:A:C8	2.54	0.42
22:23:2064:C:H2'	22:23:2065:C:C6	2.54	0.42
26:LC:52:THR:HG22	26:LC:80:TRP:CZ3	2.55	0.42
29:LF:133:LEU:HB3	29:LF:141:ILE:HD11	2.01	0.42
58:Pt:3:C:H2'	58:Pt:4:C:C6	2.54	0.42
1:16:17:U:H2'	1:16:18:C:C6	2.54	0.42
1:16:269:C:H2'	1:16:270:A:H8	1.82	0.42
1:16:512:U:H2'	1:16:513:C:C6	2.54	0.42
1:16:1009:U:H2'	1:16:1010:U:H6	1.84	0.42
2:SB:4:VAL:HG13	2:SB:4:VAL:O	2.19	0.42
3:SC:42:TYR:HA	3:SC:45:LYS:NZ	2.35	0.42
22:23:286:U:H2'	22:23:287:G:C8	2.55	0.42
25:LB:201:MET:HE3	25:LB:201:MET:HB2	1.81	0.42
56:EF:104:ARG:HH21	56:EF:295:ILE:HD11	1.85	0.42
1:16:1120:C:H2'	1:16:1121:U:C6	2.55	0.42
5:SE:60:ILE:O	5:SE:64:MET:HG2	2.18	0.42
9:SI:9:THR:H	9:SI:85:ARG:HD2	1.84	0.42
13:SM:54:ASP:OD1	13:SM:55:THR:N	2.52	0.42
22:23:158:U:H1'	22:23:169:G:N2	2.34	0.42
28:LE:65:PRO:HA	28:LE:89:VAL:HG22	2.02	0.42
1:16:1218:C:H2'	1:16:1219:A:C8	2.55	0.42
1:16:1254:A:H2'	1:16:1255:G:C8	2.54	0.42
1:16:1451:U:H3'	1:16:1452:C:H6	1.84	0.42
22:23:413:C:H2'	22:23:414:C:C6	2.55	0.42
22:23:629:G:H5"	22:23:650:C:O2'	2.20	0.42
22:23:2177:C:H2'	22:23:2178:C:C6	2.55	0.42
22:23:2557:G:H2'	22:23:2558:C:C6	2.54	0.42
22:23:2591:C:H2'	22:23:2592:G:C8	2.55	0.42
24:LA:27:ILE:CG2	24:LA:182:ALA:HB1	2.50	0.42
27:LD:31:VAL:HG22	27:LD:96:VAL:HG11	2.01	0.42
31:LJ:42:ARG:NH2	31:LJ:54:VAL:HG23	2.34	0.42
56:EF:309:ARG:HB2	56:EF:404:ILE:HD12	2.00	0.42
56:EF:518:VAL:HG13	56:EF:578:LEU:HD13	2.02	0.42
4:SD:107:PHE:HB3	4:SD:145:ILE:HD13	2.00	0.42
22:23:2181:U:H2'	22:23:2182:U:C6	2.54	0.42
23:5:15:A:H3'	23:5:16:G:H8	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:LC:40:LEU:HG	26:LC:46:ARG:HG3	2.02	0.42
56:EF:76:ALA:HB2	56:EF:202:PHE:CZ	2.54	0.42
1:16:922:G:H2'	1:16:923:A:C8	2.54	0.42
19:SS:17:LYS:O	19:SS:20:GLU:HG3	2.20	0.42
22:23:308:G:H2'	22:23:309:A:C8	2.55	0.42
22:23:666:A:H2'	22:23:667:U:C6	2.55	0.42
22:23:1438:U:H2'	22:23:1439:A:C8	2.54	0.42
22:23:1735:A:H2'	22:23:1736:U:C6	2.54	0.42
22:23:2637:U:H2'	22:23:2638:G:O4'	2.19	0.42
29:LF:52:PHE:CE2	29:LF:72:LEU:HD22	2.55	0.42
34:LN:113:MET:HE2	34:LN:113:MET:HA	2.02	0.42
54:Li:16:LYS:HE2	54:Li:20:GLY:HA2	2.02	0.42
1:16:262:A:H2'	1:16:263:A:C8	2.55	0.42
1:16:738:C:H2'	1:16:739:C:C6	2.55	0.42
1:16:859:G:H2'	1:16:860:A:C8	2.55	0.42
11:SK:15:GLN:HA	11:SK:77:TYR:O	2.20	0.42
22:23:1324:G:H1'	22:23:1616:A:N6	2.35	0.42
22:23:2106:U:H2'	22:23:2107:G:C8	2.55	0.42
22:23:2159:G:H2'	22:23:2160:C:C6	2.55	0.42
24:LA:7:ARG:O	24:LA:11:ILE:HG13	2.19	0.42
34:LN:58:LEU:HD11	34:LN:86:LEU:HD13	2.01	0.42
56:EF:135:VAL:O	56:EF:137:ARG:HG3	2.19	0.42
56:EF:193:TRP:HZ2	56:EF:277:ALA:HB2	1.84	0.42
57:Dt:70:C:H2'	57:Dt:71:G:H8	1.85	0.42
22:23:554:U:H2'	22:23:555:G:O4'	2.20	0.42
22:23:813:U:H2'	22:23:814:C:C6	2.55	0.42
22:23:828:U:H2'	22:23:829:A:C8	2.55	0.42
22:23:2660:A:H2'	22:23:2661:G:O4'	2.19	0.42
56:EF:276:GLN:CD	56:EF:276:GLN:H	2.26	0.42
60:B:7:DHA:CB	60:B:8:SAR:HN1	2.18	0.42
1:16:442:G:H1	1:16:492:C:H42	1.67	0.41
1:16:1267:C:N3	1:16:1327:C:H4'	2.34	0.41
1:16:1295:U:H2'	1:16:1296:C:C6	2.55	0.41
3:SC:23:PHE:HB2	10:SJ:95:GLY:O	2.20	0.41
10:SJ:52:LEU:HB2	14:SN:81:ARG:HD2	2.02	0.41
22:23:2208:C:H2'	22:23:2209:G:C8	2.54	0.41
22:23:2385:C:H2'	22:23:2386:A:C8	2.54	0.41
1:16:730:G:C5	1:16:731:G:H1'	2.55	0.41
2:SB:54:LEU:HD21	2:SB:216:ALA:HB1	2.01	0.41
2:SB:161:LEU:HD22	2:SB:176:ALA:HB2	2.02	0.41
6:SF:4:TYR:CD2	6:SF:71:ILE:HG13	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:23:858:G:N3	22:23:2268:A:H2'	2.35	0.41
22:23:1932:A:H2'	22:23:1933:G:O4'	2.20	0.41
22:23:2443:C:HO2'	22:23:2444:G:H5'	1.85	0.41
27:LD:117:ARG:NH2	27:LD:183:PHE:O	2.52	0.41
44:LX:25:VAL:HG13	44:LX:34:VAL:HG13	2.02	0.41
54:Li:15:LYS:HB2	54:Li:23[A]:LYS:HG2	2.02	0.41
58:Pt:22:G:H2'	58:Pt:23:A:C8	2.56	0.41
1:16:1143:G:H2'	1:16:1144:G:C8	2.56	0.41
3:SC:138:VAL:HG13	3:SC:149:ILE:HG21	2.01	0.41
22:23:1447:C:H2'	22:23:1448:G:C8	2.55	0.41
27:LD:148:ILE:HA	27:LD:187:VAL:HG13	2.02	0.41
32:LK:103:ARG:HG3	32:LK:141:GLU:HB2	2.02	0.41
56:EF:423:LYS:HD3	56:EF:482:ASN:HD21	1.84	0.41
1:16:717:U:H4'	11:SK:119:ASN:ND2	2.35	0.41
14:SN:43:ASN:HB3	14:SN:47:LYS:NZ	2.35	0.41
22:23:3:U:H2'	22:23:4:U:C6	2.55	0.41
22:23:397:U:H5"	47:Lb:32:ASN:HB2	2.03	0.41
22:23:482:A:H1'	22:23:498:G:N2	2.35	0.41
22:23:609:A:H2'	22:23:610:C:O4'	2.21	0.41
22:23:1434:A:H2'	22:23:1435:G:C8	2.56	0.41
25:LB:87:ARG:HG3	25:LB:89:ALA:O	2.20	0.41
33:LM:19:ASP:O	33:LM:23:LYS:HE2	2.20	0.41
56:EF:509:SER:HA	58:Pt:37:MIA:H4'	2.03	0.41
1:16:1008:U:H2'	1:16:1009:U:C6	2.55	0.41
7:SG:104:ILE:HA	7:SG:134:ALA:HB2	2.02	0.41
22:23:320:A:H4'	22:23:322:A:N7	2.36	0.41
32:LK:130:GLU:HB2	32:LK:140:VAL:HG21	2.01	0.41
40:LT:16:LYS:HE2	40:LT:16:LYS:HB3	1.86	0.41
56:EF:448:TRP:NE1	60:B:6:DBB:HG1	2.35	0.41
1:16:948:C:H2'	1:16:949:A:H8	1.85	0.41
2:SB:129:LEU:C	2:SB:131:LYS:H	2.28	0.41
9:SI:113:ARG:HD2	14:SN:101:TRP:C	2.46	0.41
13:SM:4:ILE:HG12	13:SM:5:ALA:H	1.86	0.41
22:23:596:U:H2'	22:23:597:G:C8	2.56	0.41
22:23:639:U:H2'	22:23:640:C:C6	2.56	0.41
28:LE:8:TYR:HA	28:LE:12:VAL:HB	2.03	0.41
32:LK:59:ILE:HD13	32:LK:69:PHE:HB3	2.01	0.41
32:LK:108:GLU:HG2	32:LK:109:ILE:N	2.35	0.41
34:LN:104:THR:C	34:LN:106:GLU:H	2.27	0.41
56:EF:17:ALA:HB3	56:EF:23:LYS:HG3	2.01	0.41
56:EF:171:LEU:HD11	56:EF:218:TRP:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:mR:43:A:H2'	59:mR:44:A:C8	2.56	0.41
7:SG:44:TYR:O	7:SG:47:LEU:HG	2.21	0.41
10:SJ:25:ILE:HD11	10:SJ:74:VAL:HG21	2.01	0.41
22:23:703:U:H2'	22:23:704:G:O4'	2.21	0.41
22:23:753:A:H2'	22:23:754:U:C6	2.56	0.41
22:23:885:C:H2'	22:23:886:A:C8	2.55	0.41
22:23:1830:C:H2'	22:23:1831:G:H8	1.86	0.41
22:23:2121:G:H2'	22:23:2122:U:H6	1.86	0.41
22:23:2313:C:H2'	22:23:2314:A:C8	2.56	0.41
22:23:2649:C:H2'	22:23:2650:U:C6	2.56	0.41
56:EF:302:GLY:C	56:EF:304:ASP:H	2.29	0.41
56:EF:488:VAL:HA	60:B:2:BB9:SG	2.60	0.41
1:16:191:G:H2'	1:16:192:A:C8	2.55	0.41
1:16:474:G:H2'	1:16:475:C:C6	2.56	0.41
1:16:920:U:H2'	1:16:921:U:C6	2.55	0.41
22:23:27:G:H22	22:23:512:G:H1'	1.84	0.41
22:23:1057:A:N7	22:23:1086:A:H2'	2.35	0.41
22:23:1064:C:H2'	22:23:1065:U:O4'	2.20	0.41
22:23:1082:U:H5'	32:LK:119:GLY:CA	2.48	0.41
33:LM:28:LEU:CD1	33:LM:142:ILE:HD12	2.50	0.41
36:LP:90:GLU:OE1	36:LP:90:GLU:HA	2.21	0.41
56:EF:495:ARG:O	56:EF:496:GLN:HB2	2.20	0.41
1:16:6:G:H1	5:SE:103:THR:HG21	1.86	0.41
1:16:234:C:H2'	1:16:235:C:C6	2.56	0.41
1:16:779:C:H2'	1:16:780:A:O4'	2.21	0.41
1:16:878:A:H1'	8:SH:4:GLN:HG3	2.02	0.41
1:16:1435:G:H2'	1:16:1436:U:C6	2.55	0.41
1:16:1476:A:H2'	1:16:1477:U:H6	1.83	0.41
4:SD:116:GLN:HG2	4:SD:154:ARG:HH12	1.85	0.41
7:SG:67:GLU:HA	7:SG:70:ARG:HB2	2.03	0.41
7:SG:100:ALA:O	7:SG:104:ILE:HG13	2.20	0.41
19:SS:50:ALA:HA	19:SS:59:PRO:HA	2.02	0.41
22:23:581:C:H2'	22:23:582:A:C8	2.55	0.41
22:23:785:G:H2'	22:23:786:C:C6	2.55	0.41
22:23:857:G:H2'	22:23:858:G:O4'	2.21	0.41
22:23:1443:U:H2'	22:23:1444:G:C8	2.56	0.41
22:23:1636:U:H2'	22:23:1637:A:C8	2.55	0.41
22:23:1736:U:H2'	22:23:1737:G:O4'	2.21	0.41
22:23:2758:A:C2	29:LF:71:LEU:HD11	2.56	0.41
22:23:2898:U:H2'	22:23:2899:A:H8	1.85	0.41
26:LC:121:THR:HB	26:LC:127:PHE:CD2	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:LE:130:MET:HG3	28:LE:154:ILE:HB	2.03	0.41
31:LJ:85:SER:HB3	31:LJ:92:ALA:HB2	2.02	0.41
38:LR:81:ARG:O	38:LR:84:GLU:HG3	2.21	0.41
56:EF:104:ARG:HH12	56:EF:407:GLU:HG2	1.86	0.41
57:Dt:67:C:H2'	57:Dt:68:C:C6	2.55	0.41
1:16:1275:A:H2'	1:16:1276:G:O4'	2.21	0.41
1:16:1363:A:H2'	1:16:1363:A:N3	2.36	0.41
1:16:1527:U:C5	21:SU:42:THR:HG21	2.56	0.41
9:SI:12:ARG:HG3	9:SI:13:LYS:HG3	2.03	0.41
14:SN:14:VAL:HA	14:SN:60:GLN:NE2	2.36	0.41
22:23:288:U:H2'	22:23:289:G:C8	2.56	0.41
22:23:2093:G:N7	22:23:2225:A:H2'	2.36	0.41
22:23:2825:G:H3'	22:23:2826:A:H8	1.86	0.41
22:23:2899:A:H2'	22:23:2900:A:C8	2.56	0.41
26:LC:1:MET:HE3	26:LC:205:PRO:HG2	2.03	0.41
30:LI:99:ILE:O	30:LI:103:VAL:HG23	2.21	0.41
38:LR:49:VAL:HG21	38:LR:82:ALA:HA	2.02	0.41
45:LY:6:ALA:HB2	45:LY:42:LEU:CD2	2.51	0.41
1:16:1261:A:H1'	1:16:1283:U:H5"	2.04	0.40
22:23:28:A:H1'	22:23:513:A:C2	2.56	0.40
22:23:588:U:H2'	22:23:589:U:C6	2.56	0.40
22:23:878:A:H3'	22:23:879:G:H8	1.87	0.40
22:23:1173:U:H2'	22:23:1174:U:O4'	2.21	0.40
22:23:1605:C:H2'	22:23:1606:C:O4'	2.21	0.40
22:23:1927:A:H2'	22:23:1928:A:C8	2.56	0.40
33:LM:16:TYR:HA	33:LM:138:GLN:O	2.20	0.40
34:LN:7:MET:HE3	34:LN:7:MET:HB3	1.84	0.40
46:La:41:ARG:HD3	46:La:41:ARG:HA	1.82	0.40
1:16:1048:G:H2'	1:16:1050:G:H8	1.85	0.40
22:23:160:A:H2'	22:23:161:A:C8	2.56	0.40
22:23:1190:G:H5"	35:LO:32:GLY:HA2	2.02	0.40
22:23:1645:G:H5"	22:23:1646:C:H5'	2.02	0.40
22:23:1808:A:H3'	22:23:1809:A:C8	2.56	0.40
22:23:2036:C:H2'	22:23:2037:A:C8	2.55	0.40
29:LF:44:LYS:HB2	29:LF:51:THR:HG1	1.86	0.40
33:LM:110:PRO:O	33:LM:115:GLY:HA3	2.21	0.40
42:LV:46:LEU:O	42:LV:50:VAL:HG23	2.19	0.40
48:Lc:50:VAL:O	48:Lc:53:VAL:HG12	2.21	0.40
58:Pt:51:U:H3	58:Pt:63:G:H1	1.70	0.40
58:Pt:67:C:H2'	58:Pt:68:C:C6	2.57	0.40
1:16:516:PSU:H2'	1:16:517:G:C8	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:16:780:A:H5”	11:SK:125:LYS:HD3	2.03	0.40
1:16:1141:C:H2’	1:16:1142:G:H8	1.86	0.40
1:16:1187:G:H2’	1:16:1188:A:C8	2.56	0.40
13:SM:115:PRO:O	13:SM:116:ILE:C	2.64	0.40
19:SS:18:LYS:HE3	19:SS:31:LEU:HD21	2.03	0.40
22:23:106:C:H2’	22:23:107:G:C8	2.56	0.40
22:23:1224:U:H4’	41:LU:88:GLY:O	2.21	0.40
22:23:1353:A:H2’	22:23:1354:A:C8	2.56	0.40
22:23:2774:C:H2’	22:23:2775:G:O4’	2.22	0.40
56:EF:605:PHE:CE2	56:EF:610:PRO:HB3	2.55	0.40
1:16:71:A:H61	1:16:99:C:H1’	1.86	0.40
1:16:1134:G:C2	1:16:1135:U:H1’	2.57	0.40
1:16:1268:G:H2’	1:16:1269:A:C8	2.56	0.40
22:23:679:C:H2’	22:23:680:C:C6	2.56	0.40
22:23:1877:A:H2’	22:23:1878:G:O4’	2.21	0.40
22:23:2121:G:H2’	22:23:2122:U:C6	2.56	0.40
22:23:2896:C:H2’	22:23:2897:U:C6	2.57	0.40
25:LB:155:ALA:HB2	25:LB:162:VAL:HG23	2.04	0.40
27:LD:188:MET:HE1	27:LD:196:VAL:HG11	2.03	0.40
28:LE:4:LEU:HB2	28:LE:101:GLU:HB3	2.03	0.40
39:LS:29:LYS:HB3	39:LS:40:LEU:HD22	2.04	0.40
43:LW:48:GLN:HG3	43:LW:55:VAL:HG22	2.04	0.40
56:EF:186:VAL:HG13	56:EF:248:ILE:HD11	2.03	0.40
56:EF:487:GLN:O	60:B:1:DAL:HA	2.20	0.40
1:16:6:G:H22	5:SE:103:THR:HG22	1.85	0.40
1:16:751:U:H2’	1:16:752:G:O4’	2.21	0.40
1:16:1478:U:H2’	1:16:1479:C:C6	2.57	0.40
5:SE:23:LYS:HB3	5:SE:23:LYS:HE2	1.87	0.40
5:SE:154:ALA:HB1	5:SE:159:LYS:O	2.22	0.40
10:SJ:83:THR:O	10:SJ:87:LEU:HG	2.21	0.40
22:23:713:G:H2’	22:23:714:U:C6	2.57	0.40
22:23:2079:U:H2’	22:23:2080:A:O4’	2.21	0.40
24:LA:46:VAL:HG22	24:LA:212:VAL:HG13	2.03	0.40
35:LO:27:LEU:O	35:LO:31:GLY:HA2	2.22	0.40
57:Dt:12:G:H1	57:Dt:24:C:H42	1.69	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	
2	SB	224/241 (93%)	214 (96%)	10 (4%)	0	100	100
3	SC	204/233 (88%)	196 (96%)	8 (4%)	0	100	100
4	SD	203/206 (98%)	197 (97%)	5 (2%)	1 (0%)	24	44
5	SE	153/167 (92%)	148 (97%)	5 (3%)	0	100	100
6	SF	104/135 (77%)	100 (96%)	4 (4%)	0	100	100
7	SG	154/179 (86%)	145 (94%)	9 (6%)	0	100	100
8	SH	127/130 (98%)	124 (98%)	2 (2%)	1 (1%)	16	32
9	SI	125/130 (96%)	120 (96%)	5 (4%)	0	100	100
10	SJ	97/103 (94%)	93 (96%)	4 (4%)	0	100	100
11	SK	115/129 (89%)	110 (96%)	4 (4%)	1 (1%)	14	29
12	SL	120/124 (97%)	113 (94%)	6 (5%)	1 (1%)	16	32
13	SM	113/118 (96%)	108 (96%)	5 (4%)	0	100	100
14	SN	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
15	SO	86/89 (97%)	86 (100%)	0	0	100	100
16	SP	80/82 (98%)	79 (99%)	1 (1%)	0	100	100
17	SQ	78/84 (93%)	74 (95%)	4 (5%)	0	100	100
18	SR	65/75 (87%)	62 (95%)	3 (5%)	0	100	100
19	SS	82/92 (89%)	80 (98%)	1 (1%)	1 (1%)	10	22
20	ST	84/87 (97%)	84 (100%)	0	0	100	100
21	SU	68/71 (96%)	66 (97%)	2 (3%)	0	100	100
24	LA	130/234 (56%)	122 (94%)	8 (6%)	0	100	100
25	LB	269/273 (98%)	260 (97%)	9 (3%)	0	100	100
26	LC	207/209 (99%)	198 (96%)	9 (4%)	0	100	100
27	LD	199/201 (99%)	198 (100%)	1 (0%)	0	100	100
28	LE	175/179 (98%)	169 (97%)	6 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	LF	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
30	LI	147/149 (99%)	138 (94%)	9 (6%)	0	100	100
31	LJ	127/165 (77%)	125 (98%)	2 (2%)	0	100	100
32	LK	132/142 (93%)	132 (100%)	0	0	100	100
33	LM	141/142 (99%)	138 (98%)	3 (2%)	0	100	100
34	LN	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
35	LO	143/144 (99%)	138 (96%)	5 (4%)	0	100	100
36	LP	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
37	LQ	118/127 (93%)	114 (97%)	4 (3%)	0	100	100
38	LR	114/117 (97%)	111 (97%)	3 (3%)	0	100	100
39	LS	112/115 (97%)	108 (96%)	4 (4%)	0	100	100
40	LT	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
41	LU	101/103 (98%)	96 (95%)	5 (5%)	0	100	100
42	LV	108/110 (98%)	103 (95%)	5 (5%)	0	100	100
43	LW	91/100 (91%)	88 (97%)	3 (3%)	0	100	100
44	LX	90/104 (86%)	87 (97%)	3 (3%)	0	100	100
45	LY	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
46	La	77/85 (91%)	74 (96%)	3 (4%)	0	100	100
47	Lb	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
48	Lc	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
49	Ld	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
50	Le	65/70 (93%)	63 (97%)	2 (3%)	0	100	100
51	Lf	54/57 (95%)	54 (100%)	0	0	100	100
52	Lg	48/55 (87%)	48 (100%)	0	0	100	100
53	Lh	44/46 (96%)	44 (100%)	0	0	100	100
54	Li	63/65 (97%)	61 (97%)	2 (3%)	0	100	100
55	Lj	36/38 (95%)	36 (100%)	0	0	100	100
56	EF	668/700 (95%)	642 (96%)	24 (4%)	2 (0%)	36	56
60	B	2/8 (25%)	0	2 (100%)	0	100	100
All	All	6667/7162 (93%)	6448 (97%)	212 (3%)	7 (0%)	49	69

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	SD	122	ALA
19	SS	54	GLY
56	EF	7	ILE
8	SH	55	THR
11	SK	119	ASN
12	SL	45	PRO
56	EF	166	PRO

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	
2	SB	188/199 (94%)	187 (100%)	1 (0%)	81	91
3	SC	170/190 (90%)	168 (99%)	2 (1%)	63	82
4	SD	172/173 (99%)	167 (97%)	5 (3%)	37	63
5	SE	118/126 (94%)	112 (95%)	6 (5%)	21	43
6	SF	92/116 (79%)	86 (94%)	6 (6%)	15	33
7	SG	129/147 (88%)	129 (100%)	0	100	100
8	SH	104/105 (99%)	101 (97%)	3 (3%)	37	63
9	SI	105/107 (98%)	105 (100%)	0	100	100
10	SJ	87/90 (97%)	86 (99%)	1 (1%)	65	83
11	SK	90/99 (91%)	89 (99%)	1 (1%)	65	83
12	SL	102/103 (99%)	99 (97%)	3 (3%)	37	63
13	SM	93/96 (97%)	91 (98%)	2 (2%)	45	70
14	SN	83/84 (99%)	83 (100%)	0	100	100
15	SO	76/77 (99%)	74 (97%)	2 (3%)	40	66
16	SP	65/65 (100%)	62 (95%)	3 (5%)	24	47
17	SQ	74/78 (95%)	72 (97%)	2 (3%)	39	65
18	SR	58/65 (89%)	56 (97%)	2 (3%)	32	58
19	SS	72/79 (91%)	69 (96%)	3 (4%)	26	50
20	ST	65/66 (98%)	64 (98%)	1 (2%)	57	78

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	SU	60/61 (98%)	59 (98%)	1 (2%)	53	76
24	LA	110/181 (61%)	104 (94%)	6 (6%)	19	39
25	LB	216/218 (99%)	214 (99%)	2 (1%)	70	85
26	LC	164/164 (100%)	164 (100%)	0	100	100
27	LD	165/165 (100%)	165 (100%)	0	100	100
28	LE	148/150 (99%)	147 (99%)	1 (1%)	76	88
29	LF	137/138 (99%)	134 (98%)	3 (2%)	45	70
30	LI	114/114 (100%)	111 (97%)	3 (3%)	40	66
31	LJ	98/123 (80%)	95 (97%)	3 (3%)	35	60
32	LK	104/110 (94%)	103 (99%)	1 (1%)	68	84
33	LM	117/116 (101%)	114 (97%)	3 (3%)	40	66
34	LN	104/104 (100%)	101 (97%)	3 (3%)	37	63
35	LO	104/103 (101%)	104 (100%)	0	100	100
36	LP	108/108 (100%)	108 (100%)	0	100	100
37	LQ	100/103 (97%)	100 (100%)	0	100	100
38	LR	86/87 (99%)	84 (98%)	2 (2%)	44	69
39	LS	99/100 (99%)	99 (100%)	0	100	100
40	LT	89/90 (99%)	88 (99%)	1 (1%)	65	83
41	LU	84/84 (100%)	83 (99%)	1 (1%)	63	82
42	LV	93/93 (100%)	92 (99%)	1 (1%)	65	83
43	LW	80/84 (95%)	80 (100%)	0	100	100
44	LX	76/85 (89%)	76 (100%)	0	100	100
45	LY	78/78 (100%)	75 (96%)	3 (4%)	29	54
46	La	59/63 (94%)	58 (98%)	1 (2%)	53	76
47	Lb	67/68 (98%)	67 (100%)	0	100	100
48	Lc	54/55 (98%)	54 (100%)	0	100	100
49	Ld	48/49 (98%)	47 (98%)	1 (2%)	47	71
50	Le	60/62 (97%)	58 (97%)	2 (3%)	33	59
51	Lf	47/48 (98%)	45 (96%)	2 (4%)	26	49
52	Lg	45/49 (92%)	45 (100%)	0	100	100
53	Lh	38/38 (100%)	37 (97%)	1 (3%)	40	66

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	Li	52/52 (100%)	52 (100%)	0	100	100
55	Lj	34/34 (100%)	34 (100%)	0	100	100
56	EF	547/576 (95%)	512 (94%)	35 (6%)	16	33
60	B	1/1 (100%)	1 (100%)	0	100	100
All	All	5529/5819 (95%)	5410 (98%)	119 (2%)	45	70

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	SB	196	VAL
3	SC	11	ARG
3	SC	12	LEU
4	SD	99	ASP
4	SD	105	MET
4	SD	145	ILE
4	SD	163	GLU
4	SD	173	VAL
5	SE	13	GLU
5	SE	18	VAL
5	SE	72	ILE
5	SE	85	VAL
5	SE	148	ASN
5	SE	161	VAL
6	SF	7	VAL
6	SF	39	LEU
6	SF	44	ARG
6	SF	51	ILE
6	SF	54	LEU
6	SF	92	THR
8	SH	18	GLN
8	SH	32	LEU
8	SH	101	ILE
10	SJ	71	LEU
11	SK	108	THR
12	SL	21	VAL
12	SL	24	LEU
12	SL	67	ILE
13	SM	53	ILE
13	SM	64	VAL
15	SO	2	SER
15	SO	56	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	SP	19	VAL
16	SP	36	VAL
16	SP	42	ILE
17	SQ	74	THR
17	SQ	75	LEU
18	SR	14	THR
18	SR	18	VAL
19	SS	48	THR
19	SS	51	VAL
19	SS	71	LEU
20	ST	80	THR
21	SU	2	PRO
24	LA	50	ILE
24	LA	65	LEU
24	LA	170	ILE
24	LA	172	HIS
24	LA	174	THR
24	LA	209	ILE
25	LB	228	VAL
25	LB	242	LYS
28	LE	152	LEU
29	LF	11	VAL
29	LF	25	THR
29	LF	36	THR
30	LI	2	GLN
30	LI	40	THR
30	LI	122	LEU
31	LJ	64	VAL
31	LJ	108	VAL
31	LJ	118	ILE
32	LK	140	VAL
33	LM	5	THR
33	LM	10	THR
33	LM	138	GLN
34	LN	58	LEU
34	LN	104	THR
34	LN	123	LEU
38	LR	40	ILE
38	LR	43	ASN
40	LT	31	VAL
41	LU	22	LEU
42	LV	109	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
45	LY	1	MET
45	LY	60	VAL
45	LY	61	LEU
46	La	10	THR
49	Ld	14	ILE
50	Le	32	LEU
50	Le	34	LEU
51	Lf	18	SER
51	Lf	20	ASP
53	Lh	39	ARG
56	EF	7	ILE
56	EF	10	TYR
56	EF	38	HIS
56	EF	86	ILE
56	EF	88	ASP
56	EF	116	VAL
56	EF	121	PRO
56	EF	137	ARG
56	EF	173	ILE
56	EF	178	HIS
56	EF	212	VAL
56	EF	237	TYR
56	EF	238	LEU
56	EF	262	ILE
56	EF	264	VAL
56	EF	266	CYS
56	EF	283	ILE
56	EF	284	ASP
56	EF	290	VAL
56	EF	324	ILE
56	EF	340	SER
56	EF	364	VAL
56	EF	393	THR
56	EF	404	ILE
56	EF	447	VAL
56	EF	468	ILE
56	EF	469	ILE
56	EF	488	VAL
56	EF	493	THR
56	EF	494	ILE
56	EF	512	ARG
56	EF	518	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
56	EF	520	ILE
56	EF	539	ASP
56	EF	544	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

Mol	Chain	Res	Type
2	SB	24	ASN
2	SB	51	ASN
2	SB	122	GLN
2	SB	177	ASN
2	SB	203	ASN
3	SC	6	HIS
4	SD	40	GLN
4	SD	89	ASN
4	SD	136	GLN
5	SE	89	HIS
5	SE	122	ASN
5	SE	132	ASN
5	SE	135	ASN
6	SF	46	GLN
6	SF	52	ASN
6	SF	68	GLN
7	SG	68	ASN
7	SG	142	HIS
8	SH	21	ASN
8	SH	67	GLN
9	SI	5	GLN
9	SI	50	GLN
9	SI	75	GLN
10	SJ	20	GLN
10	SJ	99	GLN
11	SK	15	GLN
11	SK	24	HIS
11	SK	40	ASN
11	SK	119	ASN
12	SL	72	HIS
14	SN	62	ASN
15	SO	28	GLN
15	SO	35	GLN
15	SO	37	ASN
16	SP	26	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	SP	29	ASN
18	SR	31	ASN
18	SR	52	GLN
19	SS	43	ASN
19	SS	53	ASN
19	SS	57	HIS
20	ST	48	GLN
20	ST	55	GLN
20	ST	61	GLN
20	ST	78	ASN
24	LA	47	ASN
24	LA	160	GLN
24	LA	168	ASN
25	LB	90	ASN
26	LC	42	ASN
26	LC	150	GLN
26	LC	173	GLN
27	LD	136	GLN
27	LD	195	GLN
29	LF	20	ASN
29	LF	73	ASN
30	LI	2	GLN
30	LI	20	ASN
30	LI	66	ASN
30	LI	128	HIS
31	LJ	103	ASN
32	LK	30	GLN
32	LK	31	GLN
32	LK	94	ASN
33	LM	136	GLN
34	LN	29	HIS
35	LO	93	ASN
35	LO	104	GLN
36	LP	13	HIS
36	LP	45	GLN
37	LQ	62	ASN
38	LR	29	HIS
38	LR	98	GLN
38	LR	100	HIS
38	LR	116	GLN
39	LS	66	ASN
40	LT	71	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
41	LU	12	HIS
42	LV	7	HIS
42	LV	9	HIS
47	Lb	36	HIS
48	Lc	39	GLN
50	Le	20	ASN
50	Le	33	ASN
50	Le	61	ASN
50	Le	65	ASN
54	Li	28	ASN
56	EF	12	ASN
56	EF	122	GLN
56	EF	129	GLN
56	EF	170	GLN
56	EF	194	ASN
56	EF	219	HIS
56	EF	221	ASN
56	EF	259	ASN
56	EF	272	ASN
56	EF	344	ASN
56	EF	428	GLN
56	EF	454	ASN
56	EF	465	HIS
56	EF	478	ASN
56	EF	482	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	16	1511/1534 (98%)	304 (20%)	41 (2%)
22	23	2902/2904 (99%)	563 (19%)	68 (2%)
23	5	119/120 (99%)	24 (20%)	3 (2%)
57	Dt	76/77 (98%)	20 (26%)	0
58	Pt	75/76 (98%)	21 (28%)	0
59	mR	9/60 (15%)	3 (33%)	0
All	All	4692/4771 (98%)	935 (19%)	112 (2%)

All (935) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	16	2	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	16	4	U
1	16	5	U
1	16	7	A
1	16	9	G
1	16	22	G
1	16	30	U
1	16	31	G
1	16	32	A
1	16	39	G
1	16	47	C
1	16	48	C
1	16	50	A
1	16	51	A
1	16	58	C
1	16	64	G
1	16	65	A
1	16	71	A
1	16	75	G
1	16	94	G
1	16	95	C
1	16	119	A
1	16	120	A
1	16	121	U
1	16	123	U
1	16	129	A
1	16	130	A
1	16	131	A
1	16	141	G
1	16	146	G
1	16	163	C
1	16	164	G
1	16	171	A
1	16	173	U
1	16	174	A
1	16	177	G
1	16	181	A
1	16	182	A
1	16	188	C
1	16	189	A
1	16	197	A
1	16	198	G
1	16	209	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	16	210	C
1	16	211	G
1	16	212	G
1	16	222	C
1	16	245	U
1	16	247	G
1	16	251	G
1	16	257	G
1	16	266	G
1	16	267	C
1	16	281	G
1	16	289	G
1	16	293	G
1	16	301	G
1	16	305	G
1	16	306	A
1	16	315	A
1	16	316	C
1	16	321	A
1	16	328	C
1	16	329	A
1	16	347	G
1	16	351	G
1	16	352	C
1	16	354	G
1	16	355	C
1	16	366	A
1	16	367	U
1	16	372	C
1	16	373	A
1	16	392	C
1	16	397	A
1	16	398	U
1	16	406	G
1	16	411	A
1	16	412	A
1	16	413	G
1	16	414	A
1	16	421	U
1	16	422	C
1	16	429	U
1	16	464	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	16	466	A
1	16	467	U
1	16	468	A
1	16	470	C
1	16	495	A
1	16	505	G
1	16	508	U
1	16	511	C
1	16	518	C
1	16	521	G
1	16	527	G7M
1	16	531	U
1	16	536	C
1	16	547	A
1	16	559	A
1	16	560	A
1	16	562	U
1	16	564	C
1	16	566	G
1	16	572	A
1	16	573	A
1	16	574	A
1	16	576	C
1	16	577	G
1	16	579	A
1	16	596	A
1	16	597	G
1	16	607	A
1	16	632	U
1	16	641	U
1	16	642	A
1	16	652	U
1	16	653	U
1	16	654	G
1	16	665	A
1	16	671	G
1	16	686	U
1	16	702	A
1	16	703	G
1	16	717	U
1	16	723	U
1	16	748	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	16	755	G
1	16	777	A
1	16	793	U
1	16	794	A
1	16	798	U
1	16	799	G
1	16	812	G
1	16	814	A
1	16	815	A
1	16	817	C
1	16	819	A
1	16	820	U
1	16	821	G
1	16	828	U
1	16	829	G
1	16	832	G
1	16	838	G
1	16	851	G
1	16	864	A
1	16	867	G
1	16	870	U
1	16	884	U
1	16	885	G
1	16	887	G
1	16	889	A
1	16	902	G
1	16	907	A
1	16	919	A
1	16	927	G
1	16	934	C
1	16	935	A
1	16	945	G
1	16	960	U
1	16	961	U
1	16	968	A
1	16	969	A
1	16	971	G
1	16	972	C
1	16	974	A
1	16	975	A
1	16	977	A
1	16	982	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	16	991	U
1	16	992	U
1	16	993	G
1	16	994	A
1	16	1004	A
1	16	1010	U
1	16	1014	A
1	16	1017	U
1	16	1025	U
1	16	1026	G
1	16	1027	C
1	16	1029	U
1	16	1030	U
1	16	1031	C
1	16	1033	G
1	16	1037	C
1	16	1038	C
1	16	1045	C
1	16	1046	A
1	16	1053	G
1	16	1054	C
1	16	1056	U
1	16	1065	U
1	16	1068	G
1	16	1070	U
1	16	1085	U
1	16	1086	U
1	16	1089	G
1	16	1094	G
1	16	1095	U
1	16	1101	A
1	16	1104	G
1	16	1124	G
1	16	1125	U
1	16	1126	U
1	16	1129	C
1	16	1130	A
1	16	1133	G
1	16	1136	C
1	16	1137	C
1	16	1139	G
1	16	1145	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	16	1146	A
1	16	1151	A
1	16	1152	A
1	16	1157	A
1	16	1159	U
1	16	1160	G
1	16	1167	A
1	16	1168	U
1	16	1169	A
1	16	1183	U
1	16	1184	G
1	16	1191	A
1	16	1195	C
1	16	1196	A
1	16	1197	A
1	16	1198	G
1	16	1200	C
1	16	1201	A
1	16	1212	U
1	16	1213	A
1	16	1214	C
1	16	1224	U
1	16	1225	A
1	16	1226	C
1	16	1238	A
1	16	1239	A
1	16	1240	U
1	16	1241	G
1	16	1249	C
1	16	1250	A
1	16	1258	G
1	16	1259	C
1	16	1260	G
1	16	1270	G
1	16	1279	G
1	16	1281	C
1	16	1282	C
1	16	1285	A
1	16	1286	U
1	16	1287	A
1	16	1288	A
1	16	1289	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	16	1290	G
1	16	1294	G
1	16	1297	G
1	16	1298	U
1	16	1299	A
1	16	1300	G
1	16	1302	C
1	16	1303	C
1	16	1305	G
1	16	1317	C
1	16	1318	A
1	16	1322	C
1	16	1336	C
1	16	1337	G
1	16	1340	A
1	16	1345	U
1	16	1346	A
1	16	1348	U
1	16	1353	G
1	16	1360	A
1	16	1363	A
1	16	1364	U
1	16	1365	G
1	16	1378	C
1	16	1379	G
1	16	1380	U
1	16	1381	U
1	16	1383	C
1	16	1396	A
1	16	1399	C
1	16	1419	G
1	16	1429	A
1	16	1432	G
1	16	1433	A
1	16	1441	A
1	16	1442	G
1	16	1446	A
1	16	1451	U
1	16	1452	C
1	16	1453	G
1	16	1454	G
1	16	1487	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	16	1492	A
1	16	1493	A
1	16	1497	G
1	16	1499	A
1	16	1503	A
1	16	1505	G
1	16	1506	U
1	16	1529	G
1	16	1530	G
22	23	10	A
22	23	33	C
22	23	34	U
22	23	36	G
22	23	51	G
22	23	58	G
22	23	63	A
22	23	71	A
22	23	73	A
22	23	74	A
22	23	75	G
22	23	80	G
22	23	91	A
22	23	101	A
22	23	102	U
22	23	118	A
22	23	119	A
22	23	120	U
22	23	125	A
22	23	126	A
22	23	139	U
22	23	140	C
22	23	142	A
22	23	160	A
22	23	163	C
22	23	165	A
22	23	177	G
22	23	178	G
22	23	181	A
22	23	196	A
22	23	199	A
22	23	200	U
22	23	215	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	23	216	A
22	23	221	A
22	23	222	A
22	23	223	A
22	23	224	U
22	23	228	C
22	23	230	G
22	23	233	A
22	23	239	C
22	23	242	G
22	23	248	G
22	23	252	G
22	23	265	A
22	23	266	G
22	23	267	C
22	23	272	A
22	23	276	U
22	23	277	G
22	23	278	A
22	23	279	A
22	23	282	A
22	23	295	G
22	23	311	A
22	23	329	G
22	23	330	A
22	23	334	C
22	23	338	G
22	23	343	C
22	23	346	A
22	23	361	G
22	23	362	A
22	23	369	U
22	23	370	G
22	23	372	G
22	23	380	G
22	23	383	C
22	23	386	G
22	23	396	G
22	23	399	U
22	23	401	A
22	23	404	A
22	23	405	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	23	406	G
22	23	411	G
22	23	412	A
22	23	422	A
22	23	428	A
22	23	434	U
22	23	443	A
22	23	451	U
22	23	455	C
22	23	456	C
22	23	475	C
22	23	479	A
22	23	481	G
22	23	489	G
22	23	491	G
22	23	496	G
22	23	503	A
22	23	504	A
22	23	505	A
22	23	507	A
22	23	509	C
22	23	530	G
22	23	531	C
22	23	532	A
22	23	546	U
22	23	547	A
22	23	549	G
22	23	550	C
22	23	555	G
22	23	556	A
22	23	563	A
22	23	568	U
22	23	573	U
22	23	575	A
22	23	603	A
22	23	614	A
22	23	615	U
22	23	616	A
22	23	622	G
22	23	627	A
22	23	637	A
22	23	645	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	23	647	G
22	23	653	U
22	23	654	A
22	23	655	A
22	23	659	G
22	23	668	A
22	23	682	G
22	23	685	A
22	23	686	U
22	23	695	G
22	23	702	U
22	23	704	G
22	23	726	G
22	23	730	A
22	23	731	C
22	23	738	G
22	23	740	C
22	23	746	PSU
22	23	747	5MU
22	23	757	G
22	23	762	U
22	23	765	C
22	23	775	G
22	23	776	G
22	23	782	A
22	23	784	G
22	23	785	G
22	23	787	C
22	23	788	A
22	23	791	C
22	23	792	A
22	23	805	G
22	23	812	C
22	23	819	A
22	23	827	U
22	23	828	U
22	23	831	G
22	23	846	U
22	23	847	U
22	23	858	G
22	23	859	G
22	23	865	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	23	866	A
22	23	869	G
22	23	877	A
22	23	880	G
22	23	886	A
22	23	890	C
22	23	891	G
22	23	893	C
22	23	896	A
22	23	906	U
22	23	907	G
22	23	909	A
22	23	910	A
22	23	913	U
22	23	914	G
22	23	917	A
22	23	927	A
22	23	931	U
22	23	932	U
22	23	934	U
22	23	941	A
22	23	946	C
22	23	953	G
22	23	961	C
22	23	973	A
22	23	974	G
22	23	980	A
22	23	983	A
22	23	984	A
22	23	985	C
22	23	989	G
22	23	996	A
22	23	999	U
22	23	1009	A
22	23	1011	G
22	23	1012	U
22	23	1013	C
22	23	1022	G
22	23	1026	G
22	23	1033	U
22	23	1040	A
22	23	1047	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	23	1060	U
22	23	1069	A
22	23	1070	A
22	23	1071	G
22	23	1078	U
22	23	1084	A
22	23	1087	G
22	23	1088	A
22	23	1089	A
22	23	1096	A
22	23	1097	U
22	23	1110	G
22	23	1111	A
22	23	1112	G
22	23	1116	G
22	23	1130	U
22	23	1132	U
22	23	1133	A
22	23	1134	A
22	23	1135	C
22	23	1139	G
22	23	1141	U
22	23	1142	A
22	23	1148	U
22	23	1156	A
22	23	1174	U
22	23	1175	A
22	23	1176	U
22	23	1177	G
22	23	1206	G
22	23	1212	G
22	23	1218	G
22	23	1223	G
22	23	1227	G
22	23	1236	G
22	23	1238	G
22	23	1247	A
22	23	1248	G
22	23	1250	G
22	23	1253	A
22	23	1256	G
22	23	1262	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	23	1266	G
22	23	1267	U
22	23	1271	G
22	23	1272	A
22	23	1275	A
22	23	1288	G
22	23	1289	C
22	23	1300	G
22	23	1301	A
22	23	1302	A
22	23	1306	C
22	23	1320	C
22	23	1329	U
22	23	1332	G
22	23	1344	U
22	23	1345	C
22	23	1351	C
22	23	1359	A
22	23	1360	G
22	23	1365	A
22	23	1368	G
22	23	1374	G
22	23	1378	A
22	23	1379	U
22	23	1383	A
22	23	1386	C
22	23	1395	A
22	23	1413	A
22	23	1416	G
22	23	1417	C
22	23	1420	A
22	23	1421	G
22	23	1427	A
22	23	1428	C
22	23	1435	G
22	23	1449	G
22	23	1451	C
22	23	1452	G
22	23	1453	A
22	23	1458	U
22	23	1478	G
22	23	1482	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	23	1493	C
22	23	1494	A
22	23	1508	A
22	23	1509	A
22	23	1515	A
22	23	1524	G
22	23	1529	G
22	23	1534	U
22	23	1536	C
22	23	1537	G
22	23	1538	G
22	23	1558	C
22	23	1566	A
22	23	1567	G
22	23	1569	A
22	23	1578	U
22	23	1583	A
22	23	1584	U
22	23	1607	C
22	23	1608	A
22	23	1609	A
22	23	1610	A
22	23	1615	C
22	23	1616	A
22	23	1617	C
22	23	1618	6MZ
22	23	1619	G
22	23	1634	A
22	23	1635	A
22	23	1647	U
22	23	1648	U
22	23	1649	G
22	23	1651	G
22	23	1654	A
22	23	1667	G
22	23	1674	G
22	23	1675	C
22	23	1693	U
22	23	1694	C
22	23	1696	G
22	23	1700	A
22	23	1707	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	23	1713	A
22	23	1715	G
22	23	1721	G
22	23	1730	C
22	23	1738	G
22	23	1744	A
22	23	1754	A
22	23	1757	A
22	23	1758	U
22	23	1764	C
22	23	1773	A
22	23	1782	U
22	23	1784	A
22	23	1786	A
22	23	1789	A
22	23	1800	C
22	23	1801	A
22	23	1808	A
22	23	1816	C
22	23	1829	A
22	23	1847	A
22	23	1857	G
22	23	1858	A
22	23	1882	U
22	23	1884	G
22	23	1900	A
22	23	1901	A
22	23	1903	G
22	23	1914	C
22	23	1919	A
22	23	1920	C
22	23	1921	G
22	23	1929	G
22	23	1930	G
22	23	1937	A
22	23	1938	A
22	23	1955	U
22	23	1963	U
22	23	1967	C
22	23	1970	A
22	23	1971	U
22	23	1972	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	23	1975	G
22	23	1980	G
22	23	1981	A
22	23	1991	U
22	23	1993	U
22	23	1997	C
22	23	2021	C
22	23	2022	U
22	23	2023	C
22	23	2030	6MZ
22	23	2031	A
22	23	2033	A
22	23	2035	G
22	23	2036	C
22	23	2043	C
22	23	2055	C
22	23	2056	G
22	23	2060	A
22	23	2061	G
22	23	2062	A
22	23	2063	C
22	23	2069	G7M
22	23	2076	U
22	23	2093	G
22	23	2111	U
22	23	2112	G
22	23	2113	U
22	23	2114	A
22	23	2115	G
22	23	2116	G
22	23	2117	A
22	23	2118	U
22	23	2119	A
22	23	2120	G
22	23	2121	G
22	23	2126	A
22	23	2127	G
22	23	2131	U
22	23	2132	U
22	23	2133	G
22	23	2134	A
22	23	2141	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	23	2144	G
22	23	2145	C
22	23	2146	C
22	23	2149	U
22	23	2157	G
22	23	2158	A
22	23	2162	G
22	23	2163	A
22	23	2164	C
22	23	2165	C
22	23	2168	G
22	23	2170	A
22	23	2171	A
22	23	2172	U
22	23	2175	C
22	23	2188	U
22	23	2198	A
22	23	2203	U
22	23	2204	G
22	23	2211	A
22	23	2212	A
22	23	2225	A
22	23	2238	G
22	23	2239	G
22	23	2251	OMG
22	23	2268	A
22	23	2278	A
22	23	2279	G
22	23	2283	C
22	23	2287	A
22	23	2288	A
22	23	2289	G
22	23	2305	U
22	23	2308	G
22	23	2309	A
22	23	2311	A
22	23	2312	U
22	23	2319	G
22	23	2320	U
22	23	2322	A
22	23	2324	U
22	23	2325	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	23	2333	A
22	23	2334	U
22	23	2335	A
22	23	2336	A
22	23	2343	U
22	23	2345	G
22	23	2347	C
22	23	2350	C
22	23	2361	G
22	23	2383	G
22	23	2385	C
22	23	2389	G
22	23	2391	G
22	23	2396	G
22	23	2402	U
22	23	2403	C
22	23	2406	A
22	23	2419	U
22	23	2423	U
22	23	2425	A
22	23	2426	A
22	23	2428	G
22	23	2429	G
22	23	2430	A
22	23	2434	A
22	23	2436	G
22	23	2441	U
22	23	2444	G
22	23	2448	A
22	23	2459	A
22	23	2468	A
22	23	2469	A
22	23	2473	U
22	23	2476	A
22	23	2484	G
22	23	2487	G
22	23	2491	U
22	23	2494	G
22	23	2498	OMC
22	23	2502	G
22	23	2505	G
22	23	2517	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	23	2518	A
22	23	2520	C
22	23	2529	G
22	23	2542	A
22	23	2547	A
22	23	2549	G
22	23	2554	U
22	23	2566	A
22	23	2567	G
22	23	2569	G
22	23	2573	C
22	23	2574	G
22	23	2582	G
22	23	2586	U
22	23	2595	G
22	23	2599	G
22	23	2602	A
22	23	2609	U
22	23	2613	U
22	23	2615	U
22	23	2629	U
22	23	2630	G
22	23	2636	C
22	23	2639	A
22	23	2645	G
22	23	2646	C
22	23	2660	A
22	23	2661	G
22	23	2663	G
22	23	2666	C
22	23	2681	C
22	23	2682	A
22	23	2684	U
22	23	2687	U
22	23	2689	U
22	23	2690	U
22	23	2691	C
22	23	2707	U
22	23	2714	G
22	23	2718	G
22	23	2720	U
22	23	2726	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	23	2728	U
22	23	2729	G
22	23	2732	G
22	23	2733	A
22	23	2744	G
22	23	2748	A
22	23	2757	A
22	23	2765	A
22	23	2778	A
22	23	2779	U
22	23	2791	G
22	23	2797	U
22	23	2800	A
22	23	2809	A
22	23	2818	U
22	23	2820	A
22	23	2835	A
22	23	2836	U
22	23	2861	U
22	23	2873	A
22	23	2874	C
22	23	2879	A
22	23	2883	A
22	23	2884	U
22	23	2885	G
22	23	2886	A
23	5	13	G
23	5	16	G
23	5	24	G
23	5	25	U
23	5	35	C
23	5	36	C
23	5	40	U
23	5	41	G
23	5	44	G
23	5	45	A
23	5	51	G
23	5	53	A
23	5	56	G
23	5	57	A
23	5	58	A
23	5	66	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	5	67	G
23	5	68	C
23	5	88	C
23	5	89	U
23	5	90	C
23	5	99	A
23	5	108	A
23	5	109	A
57	Dt	7	G
57	Dt	9	G
57	Dt	10	G
57	Dt	11	A
57	Dt	14	A
57	Dt	17	C
57	Dt	18	C
57	Dt	19	G
57	Dt	20	G
57	Dt	21	H2U
57	Dt	22	A
57	Dt	45	A
57	Dt	48	U
57	Dt	57	C
57	Dt	58	A
57	Dt	59	A
57	Dt	60	A
57	Dt	62	C
57	Dt	64	G
57	Dt	77	A
58	Pt	2	C
58	Pt	6	G
58	Pt	7	A
58	Pt	8	4SU
58	Pt	9	A
58	Pt	10	G
58	Pt	13	C
58	Pt	16	H2U
58	Pt	17	C
58	Pt	18	G
58	Pt	20	U
58	Pt	22	G
58	Pt	45	U
58	Pt	46	G7M

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
58	Pt	47	3AU
58	Pt	48	C
58	Pt	57	G
58	Pt	59	U
58	Pt	60	U
58	Pt	61	C
58	Pt	62	C
59	mR	37	A
59	mR	41	U
59	mR	43	A

All (112) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	16	30	U
1	16	64	G
1	16	70	U
1	16	129	A
1	16	181	A
1	16	305	G
1	16	315	A
1	16	327	A
1	16	421	U
1	16	428	G
1	16	438	U
1	16	466	A
1	16	467	U
1	16	562	U
1	16	575	G
1	16	641	U
1	16	702	A
1	16	721	G
1	16	884	U
1	16	934	C
1	16	991	U
1	16	993	G
1	16	1045	C
1	16	1049	U
1	16	1124	G
1	16	1129	C
1	16	1145	A
1	16	1167	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	16	1190	G
1	16	1196	A
1	16	1200	C
1	16	1224	U
1	16	1239	A
1	16	1281	C
1	16	1298	U
1	16	1345	U
1	16	1380	U
1	16	1396	A
1	16	1400	C
1	16	1432	G
1	16	1451	U
22	23	33	C
22	23	125	A
22	23	177	G
22	23	199	A
22	23	215	G
22	23	265	A
22	23	277	G
22	23	361	G
22	23	372	G
22	23	434	U
22	23	446	G
22	23	455	C
22	23	503	A
22	23	504	A
22	23	512	G
22	23	555	G
22	23	685	A
22	23	784	G
22	23	792	A
22	23	827	U
22	23	865	C
22	23	984	A
22	23	1069	A
22	23	1070	A
22	23	1083	U
22	23	1088	A
22	23	1089	A
22	23	1133	A
22	23	1204	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	23	1266	G
22	23	1288	G
22	23	1300	G
22	23	1344	U
22	23	1451	C
22	23	1454	C
22	23	1458	U
22	23	1460	U
22	23	1493	C
22	23	1607	C
22	23	1608	A
22	23	1609	A
22	23	1615	C
22	23	1647	U
22	23	1730	C
22	23	1738	G
22	23	1799	G
22	23	1847	A
22	23	1857	G
22	23	1900	A
22	23	1980	G
22	23	2111	U
22	23	2113	U
22	23	2118	U
22	23	2145	C
22	23	2162	G
22	23	2282	G
22	23	2307	G
22	23	2311	A
22	23	2319	G
22	23	2324	U
22	23	2430	A
22	23	2468	A
22	23	2517	C
22	23	2581	G
22	23	2645	G
22	23	2681	C
22	23	2756	U
22	23	2873	A
23	5	24	G
23	5	88	C
23	5	108	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	UR3	16	1498	1	19,22,23	0.96	0	26,32,35	1.84	3 (11%)
22	PSU	23	2504	22	18,21,22	1.48	4 (22%)	21,30,33	2.21	5 (23%)
22	OMU	23	2552	22,62	19,22,23	1.29	3 (15%)	25,31,34	1.99	5 (20%)
58	PSU	Pt	39	58	18,21,22	1.36	2 (11%)	21,30,33	2.07	4 (19%)
1	MA6	16	1518	1	23,26,27	1.52	5 (21%)	33,38,41	2.15	11 (33%)
58	G7M	Pt	46	58	23,26,27	2.38	5 (21%)	34,39,42	3.20	12 (35%)
22	5MC	23	1962	22,62	19,22,23	1.55	3 (15%)	26,32,35	1.30	2 (7%)
1	4OC	16	1402	1	20,23,24	0.79	0	25,32,35	1.09	1 (4%)
12	D2T	SL	89	12	8,9,10	3.34	2 (25%)	6,11,13	2.06	2 (33%)
60	BB9	B	2	60	2,5,6	3.25	1 (50%)	1,5,7	4.02	1 (100%)
57	PSU	Dt	56	57	18,21,22	1.43	2 (11%)	21,30,33	2.10	3 (14%)
22	PSU	23	1911	22	18,21,22	1.41	3 (16%)	21,30,33	2.05	3 (14%)
1	G7M	16	527	1	23,26,27	2.37	5 (21%)	34,39,42	3.05	11 (32%)
1	PSU	16	516	1	18,21,22	1.42	3 (16%)	21,30,33	2.31	5 (23%)
36	4D4	LP	81	36	9,11,12	3.18	3 (33%)	7,13,15	3.43	3 (42%)
22	PSU	23	1917	22	18,21,22	1.48	3 (16%)	21,30,33	2.09	4 (19%)
22	3TD	23	1915	22	19,22,23	1.26	2 (10%)	23,32,35	2.04	3 (13%)
22	1MG	23	745	22	23,26,27	1.19	3 (13%)	33,39,42	1.72	6 (18%)
22	2MA	23	2503	22,62	22,25,26	1.53	4 (18%)	32,37,40	2.44	8 (25%)
22	OMG	23	2251	22,62,58	23,26,27	1.24	3 (13%)	32,38,41	2.10	7 (21%)
22	PSU	23	2605	22	18,21,22	1.45	4 (22%)	21,30,33	1.99	4 (19%)
58	PSU	Pt	32	58	18,21,22	1.39	3 (16%)	21,30,33	2.10	4 (19%)
58	H2U	Pt	16	58	18,21,22	1.14	3 (16%)	19,30,33	1.18	1 (5%)
1	MA6	16	1519	1	23,26,27	1.50	5 (21%)	33,38,41	2.13	11 (33%)
1	2MG	16	966	1	23,26,27	1.27	3 (13%)	33,38,41	2.25	10 (30%)
60	DHA	B	7	60	3,4,5	4.88	1 (33%)	2,4,6	4.07	2 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
58	4SU	Pt	8	58	18,21,22	1.91	5 (27%)	25,30,33	2.34	5 (20%)
60	0UO	B	4	60	16,17,18	1.53	5 (31%)	17,23,25	1.73	5 (29%)
58	3AU	Pt	47	58	24,28,29	1.05	1 (4%)	30,40,43	1.41	4 (13%)
57	4SU	Dt	8	57	18,21,22	1.88	5 (27%)	25,30,33	2.22	5 (20%)
22	5MU	23	747	22	19,22,23	1.48	6 (31%)	27,32,35	2.15	7 (25%)
58	MIA	Pt	37	58	28,31,32	2.30	7 (25%)	38,44,47	2.85	15 (39%)
22	PSU	23	2604	22	18,21,22	1.52	3 (16%)	21,30,33	2.20	5 (23%)
22	PSU	23	2457	22	18,21,22	1.57	4 (22%)	21,30,33	2.20	6 (28%)
22	6MZ	23	2030	22	22,25,26	1.48	5 (22%)	29,36,39	2.56	11 (37%)
60	DBB	B	6	60	4,5,6	0.51	0	1,5,7	0.41	0
57	G7M	Dt	47	57	23,26,27	2.36	5 (21%)	34,39,42	3.10	11 (32%)
22	5MU	23	1939	22,62	19,22,23	1.44	5 (26%)	27,32,35	2.21	6 (22%)
57	OMC	Dt	33	57	19,22,23	0.85	0	25,31,34	0.88	1 (4%)
60	SAR	B	8	60	3,4,5	1.04	0	1,3,5	1.88	0
1	2MG	16	1516	1	23,26,27	1.25	4 (17%)	33,38,41	2.33	9 (27%)
1	5MC	16	1407	1	19,22,23	1.53	3 (15%)	26,32,35	1.26	3 (11%)
22	PSU	23	746	22,62	18,21,22	1.43	3 (16%)	21,30,33	1.97	3 (14%)
22	OMC	23	2498	22,62	19,22,23	0.85	0	25,31,34	0.82	0
22	PSU	23	2580	22	18,21,22	1.52	4 (22%)	21,30,33	2.17	5 (23%)
22	G7M	23	2069	22	23,26,27	2.38	5 (21%)	34,39,42	3.11	12 (35%)
22	6MZ	23	1618	22	22,25,26	1.47	5 (22%)	29,36,39	2.20	10 (34%)
22	PSU	23	955	22	18,21,22	1.48	4 (22%)	21,30,33	2.20	3 (14%)
1	5MC	16	967	1	19,22,23	1.62	3 (15%)	26,32,35	1.75	7 (26%)
57	H2U	Dt	21	57	18,21,22	1.06	3 (16%)	19,30,33	1.52	5 (26%)
22	H2U	23	2449	22	18,21,22	1.16	3 (16%)	19,30,33	1.11	1 (5%)
22	2MG	23	1835	22	23,26,27	1.26	3 (13%)	33,38,41	2.36	10 (30%)
58	PSU	Pt	55	58	18,21,22	1.39	2 (11%)	21,30,33	2.07	3 (14%)
22	2MG	23	2445	22,62	23,26,27	1.27	4 (17%)	33,38,41	2.29	10 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UR3	16	1498	1	-	0/7/25/26	0/2/2/2
22	PSU	23	2504	22	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	OMU	23	2552	22,62	-	0/9/27/28	0/2/2/2
58	PSU	Pt	39	58	-	0/7/25/26	0/2/2/2
1	MA6	16	1518	1	-	0/11/29/30	0/3/3/3
58	G7M	Pt	46	58	-	0/7/25/26	0/3/3/3
22	5MC	23	1962	22,62	-	0/7/25/26	0/2/2/2
1	4OC	16	1402	1	-	1/9/29/30	0/2/2/2
12	D2T	SL	89	12	-	2/7/12/14	-
60	BB9	B	2	60	-	0/0/4/6	-
57	PSU	Dt	56	57	-	0/7/25/26	0/2/2/2
22	PSU	23	1911	22	-	0/7/25/26	0/2/2/2
1	G7M	16	527	1	-	2/7/25/26	0/3/3/3
1	PSU	16	516	1	-	0/7/25/26	0/2/2/2
36	4D4	LP	81	36	-	3/11/12/14	-
22	PSU	23	1917	22	-	0/7/25/26	0/2/2/2
22	3TD	23	1915	22	-	0/7/25/26	0/2/2/2
22	1MG	23	745	22	-	0/7/25/26	0/3/3/3
22	2MA	23	2503	22,62	-	2/7/25/26	0/3/3/3
22	OMG	23	2251	22,62,58	-	3/9/27/28	0/3/3/3
22	PSU	23	2605	22	-	0/7/25/26	0/2/2/2
58	PSU	Pt	32	58	-	0/7/25/26	0/2/2/2
58	H2U	Pt	16	58	-	0/7/38/39	0/2/2/2
1	MA6	16	1519	1	-	0/11/29/30	0/3/3/3
1	2MG	16	966	1	-	1/9/27/28	0/3/3/3
60	DHA	B	7	60	-	0/0/2/4	-
58	4SU	Pt	8	58	-	3/7/25/26	0/2/2/2
60	0UO	B	4	60	-	2/7/8/10	0/2/2/2
58	3AU	Pt	47	58	-	6/16/34/35	0/2/2/2
57	4SU	Dt	8	57	-	0/7/25/26	0/2/2/2
22	5MU	23	747	22	-	2/7/25/26	0/2/2/2
58	MIA	Pt	37	58	-	3/15/33/34	0/3/3/3
22	PSU	23	2604	22	-	0/7/25/26	0/2/2/2
22	PSU	23	2457	22	-	0/7/25/26	0/2/2/2
22	6MZ	23	2030	22	-	1/9/27/28	0/3/3/3
60	DBB	B	6	60	-	1/3/4/6	-
57	G7M	Dt	47	57	-	0/7/25/26	0/3/3/3
22	5MU	23	1939	22,62	-	0/7/25/26	0/2/2/2
57	OMC	Dt	33	57	-	1/9/27/28	0/2/2/2
60	SAR	B	8	60	-	1/1/2/3	-
1	2MG	16	1516	1	-	0/9/27/28	0/3/3/3
1	5MC	16	1407	1	-	0/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	PSU	23	746	22,62	-	1/7/25/26	0/2/2/2
22	OMC	23	2498	22,62	-	2/9/27/28	0/2/2/2
22	PSU	23	2580	22	-	0/7/25/26	0/2/2/2
22	G7M	23	2069	22	-	2/7/25/26	0/3/3/3
22	6MZ	23	1618	22	-	0/9/27/28	0/3/3/3
22	PSU	23	955	22	-	0/7/25/26	0/2/2/2
1	5MC	16	967	1	-	2/7/25/26	0/2/2/2
57	H2U	Dt	21	57	-	1/7/38/39	0/2/2/2
22	H2U	23	2449	22	-	0/7/38/39	0/2/2/2
22	2MG	23	1835	22	-	0/9/27/28	0/3/3/3
58	PSU	Pt	55	58	-	0/7/25/26	0/2/2/2
22	2MG	23	2445	22,62	-	1/9/27/28	0/3/3/3

All (172) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	B	7	DHA	C-CA	8.30	1.59	1.45
58	Pt	46	G7M	C8-N7	8.00	1.46	1.33
22	23	2069	G7M	C8-N7	7.74	1.46	1.33
57	Dt	47	G7M	C8-N7	7.69	1.46	1.33
1	16	527	G7M	C8-N7	7.68	1.46	1.33
36	LP	81	4D4	CZ-NE	7.49	1.47	1.33
58	Pt	37	MIA	C13-C14	6.89	1.53	1.32
58	Pt	37	MIA	C2-S10	-6.83	1.70	1.75
12	SL	89	D2T	CB-CA	-6.64	1.52	1.54
12	SL	89	D2T	CB-SB	-5.94	1.76	1.82
1	16	967	5MC	C5-C4	5.60	1.48	1.44
22	23	1962	5MC	C5-C4	5.43	1.48	1.44
1	16	1407	5MC	C5-C4	5.40	1.48	1.44
58	Pt	8	4SU	C4-S4	-5.13	1.59	1.68
57	Dt	8	4SU	C4-S4	-4.93	1.60	1.68
1	16	1518	MA6	C5-C4	4.68	1.47	1.39
1	16	527	G7M	C5-N7	-4.57	1.33	1.39
1	16	1519	MA6	C5-C4	4.52	1.47	1.39
22	23	2503	2MA	C5-C4	4.49	1.47	1.39
22	23	2069	G7M	C5-N7	-4.47	1.34	1.39
58	Pt	37	MIA	C5-C4	4.41	1.47	1.39
36	LP	81	4D4	CZ-NH2	4.41	1.47	1.32
60	B	2	BB9	C-CA	4.36	1.52	1.45
57	Dt	47	G7M	C5-N7	-4.34	1.34	1.39
22	23	1618	6MZ	C5-C4	4.30	1.46	1.39
58	Pt	46	G7M	C5-N7	-4.26	1.34	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16	527	G7M	C8-N9	4.19	1.47	1.35
57	Dt	47	G7M	C8-N9	4.16	1.46	1.35
22	23	2030	6MZ	C5-C4	4.11	1.46	1.39
22	23	2069	G7M	C8-N9	4.10	1.46	1.35
58	Pt	46	G7M	C8-N9	4.05	1.46	1.35
57	Dt	47	G7M	C5-C4	3.84	1.47	1.38
36	LP	81	4D4	CZ-NH1	3.69	1.47	1.34
57	Dt	56	PSU	C6-C5	3.68	1.39	1.35
58	Pt	46	G7M	C5-C4	3.67	1.47	1.38
22	23	2069	G7M	C5-C4	3.66	1.47	1.38
1	16	527	G7M	C5-C4	3.62	1.47	1.38
22	23	1915	3TD	C6-C5	3.54	1.39	1.35
57	Dt	8	4SU	C4-N3	-3.53	1.34	1.37
58	Pt	55	PSU	C6-C5	3.50	1.39	1.35
22	23	2457	PSU	C4-N3	-3.45	1.32	1.38
58	Pt	8	4SU	C4-N3	-3.40	1.34	1.37
22	23	2604	PSU	C6-C5	3.26	1.38	1.35
22	23	2580	PSU	C4-N3	-3.25	1.32	1.38
58	Pt	32	PSU	C6-C5	3.18	1.38	1.35
22	23	1911	PSU	C6-C5	3.18	1.38	1.35
22	23	2605	PSU	C6-C5	3.12	1.38	1.35
58	Pt	39	PSU	C6-C5	3.11	1.38	1.35
22	23	2604	PSU	C4-N3	-3.11	1.33	1.38
22	23	2504	PSU	C4-N3	-3.10	1.33	1.38
22	23	1917	PSU	C6-C5	3.10	1.38	1.35
22	23	2605	PSU	C4-N3	-3.09	1.33	1.38
22	23	2504	PSU	C6-C5	3.06	1.38	1.35
22	23	746	PSU	C4-N3	-3.05	1.33	1.38
22	23	745	1MG	C5-C4	3.03	1.47	1.38
22	23	746	PSU	C6-C5	3.03	1.38	1.35
22	23	2552	OMU	C4-N3	-3.02	1.33	1.38
1	16	516	PSU	C4-N3	-3.00	1.33	1.38
22	23	1917	PSU	C4-N3	-2.99	1.33	1.38
22	23	955	PSU	C6-C5	2.99	1.38	1.35
22	23	955	PSU	C4-N3	-2.99	1.33	1.38
22	23	1939	5MU	C4-N3	-2.98	1.33	1.38
22	23	747	5MU	C4-N3	-2.97	1.33	1.38
22	23	2251	OMG	C5-C4	2.97	1.46	1.38
1	16	516	PSU	C6-C5	2.94	1.38	1.35
58	Pt	8	4SU	C5-C4	-2.92	1.39	1.42
1	16	1518	MA6	C5-C6	2.91	1.48	1.41
22	23	1835	2MG	C5-C4	2.90	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16	1519	MA6	C5-C6	2.86	1.48	1.41
1	16	1516	2MG	C5-C4	2.85	1.46	1.38
58	Pt	16	H2U	C2-N3	-2.85	1.33	1.38
22	23	2449	H2U	C2-N3	-2.84	1.33	1.38
57	Dt	8	4SU	C5-C4	-2.84	1.39	1.42
1	16	966	2MG	C5-C4	2.83	1.46	1.38
22	23	2457	PSU	C6-C5	2.82	1.38	1.35
22	23	2445	2MG	C6-N1	-2.81	1.33	1.38
58	Pt	32	PSU	C4-N3	-2.79	1.33	1.38
22	23	2445	2MG	C5-C4	2.77	1.46	1.38
22	23	2449	H2U	C4-N3	-2.77	1.33	1.37
57	Dt	56	PSU	C4-N3	-2.77	1.33	1.38
22	23	1911	PSU	C4-N3	-2.73	1.33	1.38
22	23	1835	2MG	C6-N1	-2.69	1.33	1.38
22	23	2251	OMG	C6-N1	-2.69	1.33	1.38
58	Pt	39	PSU	C4-N3	-2.68	1.33	1.38
58	Pt	37	MIA	C5-C6	2.68	1.48	1.41
22	23	2580	PSU	C6-C5	2.66	1.38	1.35
60	B	4	0UO	C9-C10	2.66	1.55	1.50
58	Pt	55	PSU	C4-N3	-2.65	1.33	1.38
1	16	1516	2MG	C6-N1	-2.65	1.33	1.38
22	23	747	5MU	C6-C5	2.65	1.38	1.34
22	23	2503	2MA	C5-C6	2.64	1.48	1.41
1	16	966	2MG	C6-N1	-2.63	1.33	1.38
58	Pt	16	H2U	C4-N3	-2.60	1.33	1.37
22	23	1939	5MU	C2-N3	-2.60	1.33	1.38
22	23	1939	5MU	C6-C5	2.58	1.38	1.34
22	23	2457	PSU	C2-N3	-2.58	1.33	1.37
22	23	2030	6MZ	C4-N9	-2.56	1.32	1.37
22	23	2030	6MZ	C5-C6	2.55	1.48	1.41
22	23	1618	6MZ	C5-N7	-2.54	1.34	1.39
22	23	2030	6MZ	C5-N7	-2.54	1.34	1.39
22	23	2552	OMU	C2-N3	-2.54	1.33	1.38
57	Dt	21	H2U	C2-N3	-2.52	1.33	1.38
22	23	2503	2MA	C5-N7	-2.51	1.34	1.39
22	23	1915	3TD	C2-N1	-2.50	1.34	1.37
22	23	1962	5MC	C6-N1	-2.50	1.33	1.38
22	23	747	5MU	C2-N3	-2.49	1.33	1.38
1	16	527	G7M	C6-N1	-2.49	1.34	1.38
60	B	4	0UO	C14-C13	2.49	1.43	1.39
22	23	2580	PSU	C2-N3	-2.48	1.33	1.37
1	16	967	5MC	C6-N1	-2.48	1.33	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23	1618	6MZ	C5-C6	2.48	1.47	1.41
1	16	1407	5MC	C6-C5	2.47	1.38	1.34
22	23	1962	5MC	C6-C5	2.44	1.38	1.34
22	23	1939	5MU	C6-N1	-2.44	1.33	1.38
1	16	967	5MC	C6-C5	2.41	1.38	1.34
60	B	4	0UO	O3-C17	2.40	1.41	1.37
22	23	2251	OMG	C5-N7	-2.38	1.34	1.39
1	16	1519	MA6	C4-N9	-2.37	1.32	1.37
22	23	2504	PSU	C2-N3	-2.36	1.33	1.37
22	23	745	1MG	C2-N1	2.36	1.41	1.37
22	23	2069	G7M	C6-N1	-2.34	1.34	1.38
22	23	2605	PSU	C2-N3	-2.34	1.33	1.37
22	23	2604	PSU	C2-N3	-2.33	1.33	1.37
1	16	1519	MA6	C5-N7	-2.32	1.34	1.39
22	23	747	5MU	C6-N1	-2.31	1.34	1.38
58	Pt	37	MIA	C8-N7	2.30	1.36	1.31
58	Pt	47	3AU	C2-N1	2.28	1.41	1.38
22	23	746	PSU	C2-N3	-2.28	1.33	1.37
58	Pt	16	H2U	C2-N1	-2.26	1.32	1.35
22	23	2552	OMU	C5-C4	-2.26	1.38	1.43
1	16	966	2MG	C5-N7	-2.25	1.34	1.39
22	23	1835	2MG	C5-N7	-2.24	1.34	1.39
22	23	2503	2MA	C8-N7	2.23	1.36	1.31
57	Dt	47	G7M	C6-N1	-2.23	1.34	1.38
1	16	1518	MA6	C5-N7	-2.22	1.35	1.39
22	23	747	5MU	C2-N1	2.22	1.41	1.38
58	Pt	37	MIA	C5-N7	-2.21	1.35	1.39
22	23	2580	PSU	C2-N1	-2.20	1.33	1.36
60	B	4	0UO	C11-N6	-2.20	1.33	1.37
57	Dt	8	4SU	C2-N3	-2.20	1.34	1.38
60	B	4	0UO	C18-C13	-2.19	1.38	1.41
22	23	745	1MG	C5-N7	-2.19	1.34	1.39
58	Pt	46	G7M	C6-N1	-2.19	1.34	1.38
22	23	2030	6MZ	C8-N7	2.19	1.35	1.31
22	23	955	PSU	C2-N3	-2.18	1.33	1.37
58	Pt	8	4SU	C2-N3	-2.18	1.34	1.38
57	Dt	21	H2U	C2-N1	-2.17	1.32	1.35
22	23	1917	PSU	C2-N3	-2.17	1.33	1.37
1	16	1516	2MG	C4-N9	-2.16	1.32	1.38
57	Dt	21	H2U	C4-N3	-2.15	1.34	1.37
1	16	1407	5MC	C6-N1	-2.15	1.34	1.38
1	16	516	PSU	C2-N3	-2.15	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	Dt	8	4SU	C2-N1	2.14	1.41	1.38
22	23	2445	2MG	C4-N9	-2.11	1.32	1.38
58	Pt	8	4SU	C2-N1	2.11	1.41	1.38
22	23	955	PSU	C2-N1	-2.10	1.33	1.36
22	23	747	5MU	C4-C5	2.09	1.48	1.44
22	23	2445	2MG	C5-N7	-2.09	1.34	1.39
22	23	2457	PSU	C2-N1	-2.09	1.33	1.36
22	23	1618	6MZ	C4-N9	-2.08	1.33	1.37
22	23	2449	H2U	C2-N1	-2.08	1.32	1.35
22	23	1939	5MU	C4-C5	2.08	1.48	1.44
22	23	1911	PSU	C2-N1	-2.07	1.34	1.36
22	23	2605	PSU	C2-N1	-2.06	1.34	1.36
1	16	1516	2MG	C5-N7	-2.06	1.34	1.39
1	16	1518	MA6	C4-N9	-2.05	1.33	1.37
22	23	1618	6MZ	C8-N7	2.03	1.35	1.31
1	16	1519	MA6	C8-N7	2.03	1.35	1.31
22	23	2504	PSU	C2-N1	-2.03	1.34	1.36
58	Pt	37	MIA	C4-N9	-2.03	1.33	1.37
1	16	1518	MA6	C8-N7	2.01	1.35	1.31
58	Pt	32	PSU	C2-N3	-2.00	1.34	1.37

All (293) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	Pt	37	MIA	C12-C13-C14	-9.13	110.62	127.01
22	23	2503	2MA	C5-C4-N3	-8.89	117.82	127.18
22	23	2069	G7M	CN7-N7-C8	-8.43	112.03	124.79
58	Pt	46	G7M	CN7-N7-C8	-8.38	112.09	124.79
57	Dt	47	G7M	CN7-N7-C8	-8.37	112.12	124.79
1	16	527	G7M	CN7-N7-C8	-8.19	112.39	124.79
58	Pt	37	MIA	C5-C4-N3	-7.62	119.16	127.18
22	23	1835	2MG	C2-N3-C4	7.55	121.44	112.00
22	23	2445	2MG	C2-N3-C4	7.17	120.97	112.00
22	23	2030	6MZ	C9-N6-C6	-7.14	116.23	122.85
1	16	1516	2MG	C2-N3-C4	7.05	120.82	112.00
58	Pt	46	G7M	N9-C8-N7	-7.03	95.42	112.48
22	23	955	PSU	N1-C2-N3	6.99	122.55	115.17
22	23	2069	G7M	N9-C8-N7	-6.98	95.54	112.48
22	23	2457	PSU	N1-C2-N3	6.96	122.51	115.17
22	23	2504	PSU	N1-C2-N3	6.95	122.50	115.17
1	16	966	2MG	C2-N3-C4	6.94	120.68	112.00
22	23	2503	2MA	N3-C4-N9	6.93	135.78	126.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	16	516	PSU	N1-C2-N3	6.93	122.47	115.17
22	23	1915	3TD	N1-C2-N3	6.91	121.15	116.13
22	23	2604	PSU	N1-C2-N3	6.90	122.45	115.17
1	16	1498	UR3	C4-N3-C2	-6.88	119.04	124.58
1	16	527	G7M	N9-C8-N7	-6.88	95.78	112.48
57	Dt	47	G7M	N9-C8-N7	-6.87	95.81	112.48
58	Pt	46	G7M	C8-N7-C5	6.84	116.34	107.78
36	LP	81	4D4	NE-CZ-NH2	-6.70	109.18	120.67
58	Pt	8	4SU	C4-N3-C2	-6.69	120.90	127.31
22	23	2580	PSU	N1-C2-N3	6.69	122.22	115.17
58	Pt	32	PSU	N1-C2-N3	6.63	122.16	115.17
22	23	2069	G7M	C8-N7-C5	6.63	116.07	107.78
22	23	1917	PSU	N1-C2-N3	6.58	122.11	115.17
57	Dt	47	G7M	C8-N7-C5	6.49	115.89	107.78
58	Pt	39	PSU	N1-C2-N3	6.46	121.98	115.17
1	16	527	G7M	C8-N7-C5	6.44	115.84	107.78
22	23	1911	PSU	N1-C2-N3	6.42	121.94	115.17
57	Dt	56	PSU	N1-C2-N3	6.40	121.92	115.17
58	Pt	55	PSU	N1-C2-N3	6.39	121.91	115.17
22	23	746	PSU	N1-C2-N3	6.34	121.86	115.17
22	23	2251	OMG	C5-C4-N3	-6.23	118.47	128.39
22	23	1835	2MG	C5-C4-N3	-6.17	118.57	128.39
57	Dt	8	4SU	C4-N3-C2	-6.16	121.41	127.31
22	23	2605	PSU	N1-C2-N3	6.15	121.66	115.17
57	Dt	47	G7M	N9-C4-N3	6.09	138.13	125.95
1	16	966	2MG	C5-C4-N3	-5.99	118.85	128.39
58	Pt	8	4SU	C5-C4-N3	5.99	120.32	114.75
22	23	2069	G7M	N9-C4-N3	5.92	137.80	125.95
1	16	527	G7M	N9-C4-N3	5.84	137.63	125.95
22	23	1618	6MZ	C5-C4-N3	-5.83	118.69	126.72
58	Pt	46	G7M	N9-C4-N3	5.81	137.58	125.95
58	Pt	37	MIA	N3-C4-N9	5.77	134.31	126.99
22	23	2445	2MG	C5-C4-N3	-5.70	119.31	128.39
1	16	1516	2MG	C5-C4-N3	-5.65	119.39	128.39
57	Dt	8	4SU	C5-C4-N3	5.58	119.94	114.75
22	23	1939	5MU	N3-C2-N1	5.43	121.96	114.89
22	23	1939	5MU	C4-N3-C2	-5.40	120.26	127.34
22	23	747	5MU	N3-C2-N1	5.34	121.85	114.89
1	16	1518	MA6	C5-C4-N3	-5.25	119.48	126.72
22	23	2030	6MZ	C5-C4-N3	-5.25	119.48	126.72
22	23	2251	OMG	C2-N3-C4	5.21	121.27	112.30
58	Pt	46	G7M	C5-C4-N3	-5.13	118.47	128.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	16	1519	MA6	C5-C4-N3	-5.12	119.66	126.72
57	Dt	47	G7M	C5-C4-N3	-5.12	118.48	128.15
22	23	2069	G7M	C5-C4-N3	-5.05	118.62	128.15
22	23	745	1MG	C5-C4-N3	-5.04	120.37	128.39
1	16	527	G7M	C5-C4-N3	-5.03	118.64	128.15
22	23	1915	3TD	C4-N3-C2	-5.01	119.31	124.61
22	23	747	5MU	C4-N3-C2	-5.00	120.79	127.34
60	B	7	DHA	O-C-CA	-4.99	116.17	125.53
22	23	2552	OMU	C4-N3-C2	-4.93	120.49	126.61
58	Pt	8	4SU	C5-C4-S4	-4.66	118.98	124.31
58	Pt	47	3AU	C4-N3-C2	-4.64	119.21	124.66
22	23	1618	6MZ	N3-C4-N9	4.61	135.01	127.17
22	23	1939	5MU	C5-C4-N3	4.58	119.30	115.32
22	23	2251	OMG	N9-C4-N3	4.58	135.10	125.95
22	23	2030	6MZ	C6-C5-N7	4.54	137.38	132.43
22	23	2504	PSU	C4-N3-C2	-4.54	120.12	126.37
1	16	516	PSU	C4-N3-C2	-4.53	120.13	126.37
1	16	1518	MA6	C2-N1-C6	4.52	122.87	111.83
22	23	2069	G7M	C8-N9-C4	4.50	118.23	107.09
22	23	2552	OMU	N3-C2-N1	4.48	120.73	114.89
1	16	966	2MG	N9-C4-N3	4.48	134.91	125.95
57	Dt	47	G7M	C8-N9-C4	4.47	118.15	107.09
58	Pt	46	G7M	C8-N9-C4	4.46	118.14	107.09
22	23	1835	2MG	N9-C4-N3	4.45	134.85	125.95
58	Pt	46	G7M	C2-N3-C4	4.44	119.95	112.30
22	23	2069	G7M	C2-N3-C4	4.43	119.93	112.30
1	16	527	G7M	C2-N3-C4	4.40	119.87	112.30
1	16	527	G7M	C8-N9-C4	4.37	117.92	107.09
1	16	967	5MC	O2-C2-N3	-4.35	115.47	122.33
22	23	745	1MG	C2-N3-C4	4.35	121.75	111.98
22	23	955	PSU	C4-N3-C2	-4.34	120.39	126.37
57	Dt	47	G7M	C2-N3-C4	4.34	119.77	112.30
1	16	1519	MA6	C2-N1-C6	4.32	122.37	111.83
22	23	2445	2MG	N9-C4-N3	4.31	134.57	125.95
22	23	955	PSU	O2-C2-N1	-4.23	118.43	122.79
36	LP	81	4D4	NH1-CZ-NE	-4.23	109.66	119.27
1	16	1519	MA6	C4-C5-N7	-4.23	105.75	110.58
58	Pt	39	PSU	C4-N3-C2	-4.21	120.56	126.37
22	23	2580	PSU	C4-N3-C2	-4.19	120.59	126.37
58	Pt	46	G7M	C4'-O4'-C1'	-4.19	100.21	109.47
58	Pt	55	PSU	C4-N3-C2	-4.19	120.60	126.37
22	23	2457	PSU	C4-N3-C2	-4.18	120.61	126.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	Pt	32	PSU	C4-N3-C2	-4.17	120.63	126.37
57	Dt	47	G7M	CN7-N7-C5	4.16	131.99	126.80
22	23	2604	PSU	C4-N3-C2	-4.14	120.66	126.37
22	23	2069	G7M	CN7-N7-C5	4.10	131.91	126.80
1	16	1518	MA6	C4-C5-N7	-4.08	105.91	110.58
22	23	1911	PSU	C4-N3-C2	-4.07	120.76	126.37
22	23	2552	OMU	C5-C4-N3	4.06	120.48	114.80
57	Dt	56	PSU	C4-N3-C2	-4.05	120.79	126.37
22	23	1917	PSU	C4-N3-C2	-4.05	120.80	126.37
12	SL	89	D2T	CB1-SB-CB	4.02	109.60	102.36
1	16	1518	MA6	N3-C4-N9	4.02	134.01	127.17
60	B	2	BB9	O-C-CA	-4.02	120.35	125.39
1	16	527	G7M	CN7-N7-C5	3.99	131.78	126.80
22	23	747	5MU	C5-C4-N3	3.99	118.79	115.32
22	23	2605	PSU	C4-N3-C2	-3.96	120.91	126.37
22	23	2030	6MZ	N3-C4-N9	3.96	133.91	127.17
22	23	745	1MG	N9-C4-N3	3.93	133.81	125.95
57	Dt	47	G7M	C1'-N9-C8	-3.92	113.50	126.74
22	23	1911	PSU	O2-C2-N1	-3.92	118.75	122.79
1	16	516	PSU	O2-C2-N1	-3.91	118.76	122.79
57	Dt	8	4SU	N3-C2-N1	3.89	119.96	114.89
22	23	1939	5MU	C5-C6-N1	-3.89	119.09	123.31
58	Pt	37	MIA	C6-C5-N7	3.84	136.61	132.43
22	23	746	PSU	C4-N3-C2	-3.83	121.09	126.37
57	Dt	8	4SU	C5-C4-S4	-3.83	119.93	124.31
58	Pt	46	G7M	CN7-N7-C5	3.83	131.57	126.80
1	16	1516	2MG	C6-C5-N7	3.82	137.24	130.29
1	16	1516	2MG	N9-C4-N3	3.80	133.56	125.95
22	23	2030	6MZ	C2-N3-C4	3.77	121.04	111.83
22	23	1939	5MU	O4-C4-C5	-3.76	120.61	124.92
58	Pt	8	4SU	N3-C2-N1	3.76	119.79	114.89
36	LP	81	4D4	NH1-CZ-NH2	-3.76	109.38	120.07
58	Pt	37	MIA	C15-C14-C13	-3.76	111.38	122.66
22	23	747	5MU	C5-C6-N1	-3.73	119.26	123.31
58	Pt	37	MIA	C16-C14-C13	-3.73	111.46	122.66
22	23	1618	6MZ	C2-N3-C4	3.71	120.90	111.83
1	16	1519	MA6	N3-C4-N9	3.71	133.48	127.17
58	Pt	32	PSU	O2-C2-N1	-3.71	118.96	122.79
22	23	747	5MU	O4-C4-C5	-3.70	120.68	124.92
22	23	2030	6MZ	C4-C5-N7	-3.67	106.38	110.58
58	Pt	37	MIA	C4-C5-N7	-3.67	106.38	110.58
22	23	2580	PSU	O2-C2-N1	-3.65	119.02	122.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	23	2069	G7M	C1'-N9-C8	-3.64	114.45	126.74
58	Pt	39	PSU	O2-C2-N1	-3.64	119.04	122.79
22	23	2445	2MG	C6-C5-N7	3.63	136.89	130.29
1	16	1516	2MG	N1-C2-N2	3.61	120.25	116.56
22	23	1962	5MC	C5-C6-N1	-3.59	119.42	123.31
22	23	2030	6MZ	N1-C2-N3	-3.58	123.16	128.58
58	Pt	55	PSU	O2-C2-N1	-3.57	119.11	122.79
58	Pt	46	G7M	O4'-C1'-N9	3.55	116.40	108.36
22	23	2251	OMG	C2'-C1'-N9	-3.54	107.51	114.24
1	16	1518	MA6	C2-N3-C4	3.54	120.49	111.83
57	Dt	56	PSU	O2-C2-N1	-3.53	119.15	122.79
22	23	1835	2MG	N1-C2-N2	3.48	120.12	116.56
22	23	2604	PSU	O2-C2-N1	-3.48	119.20	122.79
1	16	1519	MA6	C2-N3-C4	3.48	120.32	111.83
22	23	2504	PSU	O2-C2-N1	-3.47	119.20	122.79
22	23	1835	2MG	C6-C5-N7	3.47	136.61	130.29
22	23	1917	PSU	O2-C2-N1	-3.47	119.21	122.79
58	Pt	37	MIA	C2-N3-C4	3.47	121.37	112.29
22	23	2503	2MA	C4-C5-N7	-3.46	106.63	110.58
58	Pt	46	G7M	C1'-N9-C8	-3.44	115.13	126.74
1	16	1518	MA6	N1-C2-N3	-3.43	123.39	128.58
60	B	4	0UO	O3-C17-C18	3.35	120.59	115.84
1	16	967	5MC	C1'-N1-C6	-3.33	115.66	121.15
1	16	1519	MA6	C2'-C1'-N9	-3.33	105.03	113.30
57	Dt	21	H2U	O3'-C3'-C4'	3.30	120.57	111.08
22	23	1618	6MZ	C4-C5-N7	-3.29	106.83	110.58
58	Pt	37	MIA	C11-S10-C2	-3.28	99.79	102.25
1	16	1498	UR3	C5-C4-N3	3.25	119.32	115.04
22	23	1618	6MZ	C9-N6-C6	-3.25	119.83	122.85
22	23	2457	PSU	O2-C2-N1	-3.21	119.48	122.79
1	16	527	G7M	C1'-N9-C8	-3.20	115.94	126.74
22	23	1618	6MZ	C6-C5-N7	3.19	135.90	132.43
22	23	2251	OMG	C6-C5-N7	3.18	136.09	130.29
22	23	1618	6MZ	N1-C2-N3	-3.17	123.78	128.58
22	23	2445	2MG	N1-C2-N2	3.16	119.79	116.56
1	16	966	2MG	C6-C5-N7	3.16	136.04	130.29
1	16	1519	MA6	N1-C2-N3	-3.13	123.84	128.58
22	23	2552	OMU	C2'-C1'-N1	-3.13	108.30	114.24
22	23	2457	PSU	C3'-C2'-C1'	3.12	105.37	101.69
1	16	516	PSU	C3'-C2'-C1'	3.06	105.31	101.69
1	16	967	5MC	C5-C4-N3	-3.03	118.64	121.75
60	B	4	0UO	O3-C17-C16	-3.02	119.21	124.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	23	2552	OMU	O4-C4-C5	-2.99	120.00	125.16
22	23	2030	6MZ	C4-N9-C8	2.97	108.86	105.74
22	23	746	PSU	O2-C2-N1	-2.95	119.75	122.79
1	16	967	5MC	C1'-N1-C2	2.94	124.94	118.44
22	23	2605	PSU	O2-C2-N1	-2.93	119.77	122.79
1	16	1519	MA6	C5-N7-C8	2.91	108.03	103.45
60	B	4	0UO	C19-O3-C17	-2.91	113.25	117.51
22	23	1915	3TD	C3'-C2'-C1'	2.91	105.12	101.69
1	16	1518	MA6	C5-N7-C8	2.85	107.94	103.45
60	B	7	DHA	CB-CA-N	-2.85	118.89	125.76
1	16	1516	2MG	C4-C5-N7	-2.84	106.17	110.67
1	16	1407	5MC	C5-C4-N3	-2.84	118.84	121.75
1	16	516	PSU	C5-C6-N1	-2.83	118.21	122.14
1	16	1518	MA6	C4-N9-C8	2.79	108.67	105.74
58	Pt	37	MIA	C4-N9-C8	2.79	108.67	105.74
58	Pt	47	3AU	C5-C4-N3	2.77	119.47	115.64
1	16	1516	2MG	N2-C2-N3	-2.76	117.00	120.51
1	16	1519	MA6	C4-N9-C8	2.74	108.62	105.74
22	23	1962	5MC	C5-C4-N3	-2.73	118.95	121.75
22	23	2503	2MA	C2-N1-C6	2.71	122.27	118.10
58	Pt	37	MIA	C5-N7-C8	2.66	107.64	103.45
22	23	745	1MG	C6-C5-N7	2.66	135.27	129.36
1	16	1519	MA6	C6-C5-N7	2.66	137.67	133.43
22	23	2503	2MA	N6-C6-N1	2.64	120.59	117.03
1	16	967	5MC	O4'-C1'-N1	2.64	114.34	108.36
22	23	1939	5MU	O2-C2-N1	-2.63	119.37	122.80
22	23	2580	PSU	C3'-C2'-C1'	2.62	104.78	101.69
58	Pt	37	MIA	N3-C2-N1	-2.62	122.22	127.00
1	16	1516	2MG	C2'-C1'-N9	-2.62	105.97	113.25
22	23	2030	6MZ	C5-N7-C8	2.59	107.52	103.45
58	Pt	16	H2U	C5-C4-N3	2.59	119.44	116.69
1	16	1407	5MC	C5-C6-N1	-2.59	120.51	123.31
58	Pt	37	MIA	C2-N1-C6	2.58	122.44	117.54
22	23	2503	2MA	C5-N7-C8	2.58	107.50	103.45
22	23	1835	2MG	C4-C5-N7	-2.56	106.62	110.67
22	23	1835	2MG	N2-C2-N3	-2.55	117.26	120.51
22	23	2445	2MG	CM2-N2-C2	-2.52	118.23	123.65
57	Dt	21	H2U	C5-C4-N3	2.52	119.37	116.69
1	16	966	2MG	CM2-N2-C2	-2.51	118.25	123.65
22	23	1618	6MZ	C4-N9-C8	2.49	108.35	105.74
1	16	1516	2MG	CM2-N2-C2	-2.47	118.34	123.65
57	Dt	47	G7M	O4'-C1'-N9	2.45	113.91	108.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	23	2251	OMG	C4-C5-N7	-2.44	106.80	110.67
58	Pt	8	4SU	C1'-N1-C2	2.44	121.97	117.59
1	16	967	5MC	C5-C6-N1	-2.43	120.67	123.31
1	16	966	2MG	C4-C5-N7	-2.43	106.82	110.67
1	16	527	G7M	C2'-C1'-N9	-2.41	106.53	113.25
22	23	2445	2MG	C4-C5-N7	-2.41	106.86	110.67
57	Dt	47	G7M	O6-C6-C5	-2.40	122.65	128.01
1	16	527	G7M	O6-C6-C5	-2.40	122.65	128.01
1	16	1407	5MC	O2-C2-N3	-2.39	118.56	122.33
60	B	4	0UO	C10-C11-N6	-2.38	107.69	110.31
22	23	2604	PSU	C5-C6-N1	-2.38	118.84	122.14
22	23	1618	6MZ	C5-N7-C8	2.37	107.18	103.45
1	16	1402	4OC	O2-C2-N3	-2.35	118.62	122.33
22	23	2457	PSU	C5-C6-N1	-2.35	118.88	122.14
1	16	1518	MA6	C6-C5-N7	2.35	137.18	133.43
22	23	2030	6MZ	N9-C8-N7	-2.33	110.63	113.94
1	16	966	2MG	N1-C2-N2	2.32	118.93	116.56
22	23	2069	G7M	O6-C6-C5	-2.32	122.83	128.01
1	16	1518	MA6	C2'-C1'-N9	-2.31	107.56	113.30
22	23	2503	2MA	C4-N9-C8	2.30	108.16	105.74
22	23	745	1MG	C4-C5-N7	-2.30	107.03	110.67
58	Pt	47	3AU	C10-N3-C2	2.29	121.03	117.64
1	16	1498	UR3	C3U-N3-C4	2.28	121.03	117.87
22	23	2504	PSU	C5-C6-N1	-2.28	118.98	122.14
22	23	1835	2MG	CM2-N2-C2	-2.27	118.77	123.65
1	16	1519	MA6	N9-C8-N7	-2.26	110.73	113.94
57	Dt	33	OMC	O2-C2-N3	-2.24	118.80	122.33
22	23	747	5MU	O2-C2-N1	-2.24	119.88	122.80
1	16	966	2MG	N2-C2-N3	-2.24	117.66	120.51
22	23	1835	2MG	O6-C6-C5	-2.24	120.62	126.53
22	23	2445	2MG	N2-C2-N3	-2.23	117.66	120.51
58	Pt	37	MIA	N9-C8-N7	-2.23	110.78	113.94
58	Pt	47	3AU	C1'-N1-C2	2.23	120.68	117.04
58	Pt	39	PSU	C5-C6-N1	-2.22	119.05	122.14
22	23	2445	2MG	O6-C6-C5	-2.22	120.66	126.53
1	16	966	2MG	C2-N1-C6	-2.22	121.87	124.55
22	23	2069	G7M	C2'-C3'-C4'	-2.22	98.33	102.61
22	23	2580	PSU	C5-C6-N1	-2.21	119.08	122.14
57	Dt	21	H2U	O2-C2-N1	-2.21	120.45	123.10
1	16	966	2MG	O6-C6-C5	-2.19	120.74	126.53
22	23	2449	H2U	N3-C2-N1	2.19	118.85	116.65
22	23	1618	6MZ	O3'-C3'-C2'	-2.18	104.81	111.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	Pt	46	G7M	O6-C6-C5	-2.18	123.14	128.01
22	23	2457	PSU	O2-C2-N3	-2.17	118.00	121.86
57	Dt	21	H2U	C3'-C2'-C1'	2.15	105.52	101.46
57	Dt	21	H2U	C5-C6-N1	-2.14	105.05	111.52
22	23	2251	OMG	O6-C6-C5	-2.13	120.92	126.53
12	SL	89	D2T	O-C-CA	-2.11	119.34	124.77
22	23	747	5MU	C3'-C2'-C1'	2.10	105.44	101.46
1	16	1518	MA6	N9-C8-N7	-2.10	110.96	113.94
57	Dt	8	4SU	C2'-C1'-N1	-2.09	107.42	113.25
22	23	2445	2MG	C5-C6-N1	2.08	118.55	113.25
60	B	4	0UO	C18-C10-C11	2.08	107.75	105.93
22	23	2605	PSU	C6-C5-C4	-2.06	116.78	118.17
22	23	1917	PSU	C3'-C2'-C1'	2.06	104.12	101.69
58	Pt	32	PSU	C5-C6-N1	-2.05	119.30	122.14
22	23	2604	PSU	C3'-C2'-C1'	2.04	104.10	101.69
58	Pt	37	MIA	O4'-C1'-N9	2.04	112.01	108.09
1	16	967	5MC	CM5-C5-C6	-2.03	120.10	122.85
22	23	1835	2MG	C5-C6-N1	2.02	118.39	113.25
22	23	2504	PSU	O2-C2-N3	-2.01	118.28	121.86
22	23	2503	2MA	C6-C5-N7	2.01	135.97	132.09
22	23	2069	G7M	C2'-C1'-N9	-2.00	107.68	113.25
22	23	2030	6MZ	C2-N1-C6	2.00	121.87	115.24
22	23	745	1MG	C6-C5-C4	-2.00	117.70	119.97

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	LP	81	4D4	NE-CD-CG-CB
36	LP	81	4D4	NH1-CZ-NE-CD
1	16	527	G7M	O4'-C4'-C5'-O5'
1	16	967	5MC	O4'-C1'-N1-C2
1	16	967	5MC	O4'-C1'-N1-C6
22	23	746	PSU	O4'-C1'-C5-C6
22	23	747	5MU	O4'-C4'-C5'-O5'
22	23	2251	OMG	O4'-C4'-C5'-O5'
22	23	2251	OMG	C1'-C2'-O2'-CM2
58	Pt	8	4SU	O4'-C4'-C5'-O5'
58	Pt	37	MIA	C5-C6-N6-C12
58	Pt	37	MIA	C12-C13-C14-C15
58	Pt	47	3AU	C3'-C4'-C5'-O5'
58	Pt	47	3AU	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
60	B	8	SAR	C-CA-N-CN
1	16	527	G7M	C3'-C4'-C5'-O5'
22	23	747	5MU	C3'-C4'-C5'-O5'
22	23	2498	OMC	C3'-C4'-C5'-O5'
22	23	2498	OMC	O4'-C4'-C5'-O5'
60	B	4	0UO	C16-C17-O3-C19
22	23	2251	OMG	C3'-C4'-C5'-O5'
58	Pt	8	4SU	C3'-C4'-C5'-O5'
58	Pt	47	3AU	C4'-C5'-O5'-P
60	B	4	0UO	C18-C17-O3-C19
22	23	2069	G7M	C3'-C4'-C5'-O5'
58	Pt	37	MIA	N1-C6-N6-C12
58	Pt	47	3AU	N40-C12-C13-O31
22	23	2069	G7M	O4'-C4'-C5'-O5'
58	Pt	47	3AU	N40-C12-C13-O30
60	B	6	DBB	N-CA-CB-CG
58	Pt	47	3AU	C10-C11-C12-N40
12	SL	89	D2T	CG-CB-SB-CB1
12	SL	89	D2T	SB-CB-CG-OD1
57	Dt	21	H2U	C4'-C5'-O5'-P
1	16	1402	4OC	O4'-C4'-C5'-O5'
58	Pt	8	4SU	C4'-C5'-O5'-P
57	Dt	33	OMC	C3'-C2'-O2'-CM2
22	23	2445	2MG	C3'-C4'-C5'-O5'
1	16	966	2MG	C4'-C5'-O5'-P
36	LP	81	4D4	O-C-CA-CB
22	23	2503	2MA	C4'-C5'-O5'-P
22	23	2030	6MZ	O4'-C4'-C5'-O5'
22	23	2503	2MA	O4'-C4'-C5'-O5'

There are no ring outliers.

15 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	16	1518	MA6	2	0
58	Pt	46	G7M	1	0
60	B	2	BB9	1	0
1	16	516	PSU	1	0
22	23	2251	OMG	1	0
58	Pt	16	H2U	1	0
60	B	7	DHA	3	0
58	Pt	8	4SU	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	B	4	0UO	2	0
58	Pt	37	MIA	1	0
22	23	2030	6MZ	1	0
60	B	6	DBB	2	0
57	Dt	47	G7M	1	0
57	Dt	33	OMC	1	0
60	B	8	SAR	4	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 422 ligands modelled in this entry, 406 are monoatomic - leaving 16 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
61	PUT	23	3009	-	5,5,5	0.15	0	4,4,4	0.21	0
66	FME	Pt	3001	67	8,9,10	0.55	0	8,9,11	1.52	2 (25%)
61	PUT	23	3001	-	5,5,5	0.15	0	4,4,4	0.26	0
67	PHE	Pt	3002	66,58	8,9,12	3.35	3 (37%)	3,10,15	4.30	3 (100%)
61	PUT	16	1602	-	5,5,5	0.14	0	4,4,4	0.20	0
61	PUT	23	3004	-	5,5,5	0.15	0	4,4,4	0.27	0
61	PUT	23	3007	-	5,5,5	0.15	0	4,4,4	0.22	0
61	PUT	23	3008	-	5,5,5	0.15	0	4,4,4	0.20	0
63	SPD	23	3010	-	9,9,9	0.15	0	8,8,8	0.18	0
61	PUT	23	3002	-	5,5,5	0.15	0	4,4,4	0.28	0
63	SPD	23	3011	-	9,9,9	0.15	0	8,8,8	0.25	0
61	PUT	23	3006	-	5,5,5	0.15	0	4,4,4	0.20	0
61	PUT	23	3005	-	5,5,5	0.15	0	4,4,4	0.23	0
61	PUT	23	3003	-	5,5,5	0.14	0	4,4,4	0.23	0
61	PUT	16	1601	-	5,5,5	0.14	0	4,4,4	0.21	0
65	GDP	EF	801	-	29,30,30	1.15	4 (13%)	45,47,47	1.76	5 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	PUT	23	3009	-	-	0/3/3/3	-
66	FME	Pt	3001	67	-	5/7/9/11	-
61	PUT	23	3001	-	-	0/3/3/3	-
67	PHE	Pt	3002	66,58	-	4/8/6/8	-
61	PUT	16	1602	-	-	0/3/3/3	-
61	PUT	23	3004	-	-	0/3/3/3	-
61	PUT	23	3007	-	-	0/3/3/3	-
61	PUT	23	3008	-	-	0/3/3/3	-
63	SPD	23	3010	-	-	1/7/7/7	-
61	PUT	23	3002	-	-	1/3/3/3	-
63	SPD	23	3011	-	-	0/7/7/7	-
61	PUT	23	3006	-	-	0/3/3/3	-
61	PUT	23	3005	-	-	1/3/3/3	-
61	PUT	23	3003	-	-	0/3/3/3	-
61	PUT	16	1601	-	-	0/3/3/3	-
65	GDP	EF	801	-	-	0/16/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	Pt	3002	PHE	CD1-CG	7.85	1.39	1.33
67	Pt	3002	PHE	CD2-CG	-3.76	1.39	1.47
65	EF	801	GDP	C5-C4	2.97	1.46	1.38
67	Pt	3002	PHE	CE1-CD1	-2.82	1.39	1.49
65	EF	801	GDP	C6-N1	-2.63	1.33	1.38
65	EF	801	GDP	C5-N7	-2.12	1.34	1.39
65	EF	801	GDP	C4-N9	-2.01	1.33	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
65	EF	801	GDP	C5-C4-N3	-5.73	119.27	128.39
65	EF	801	GDP	C2-N3-C4	4.90	120.73	112.30
67	Pt	3002	PHE	CB-CG-CD1	-4.66	119.27	126.41
67	Pt	3002	PHE	CE1-CD1-CG	-4.45	119.59	126.98
65	EF	801	GDP	N9-C4-N3	4.14	134.23	125.95
67	Pt	3002	PHE	CE2-CD2-CG	-3.71	119.76	126.63
65	EF	801	GDP	C6-C5-N7	3.58	136.80	130.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
66	Pt	3001	FME	CA-N-CN	-2.82	118.48	122.82
65	EF	801	GDP	C4-C5-N7	-2.63	106.50	110.67
66	Pt	3001	FME	O1-CN-N	-2.21	119.62	125.32

There are no chirality outliers.

All (12) torsion outliers are listed below:

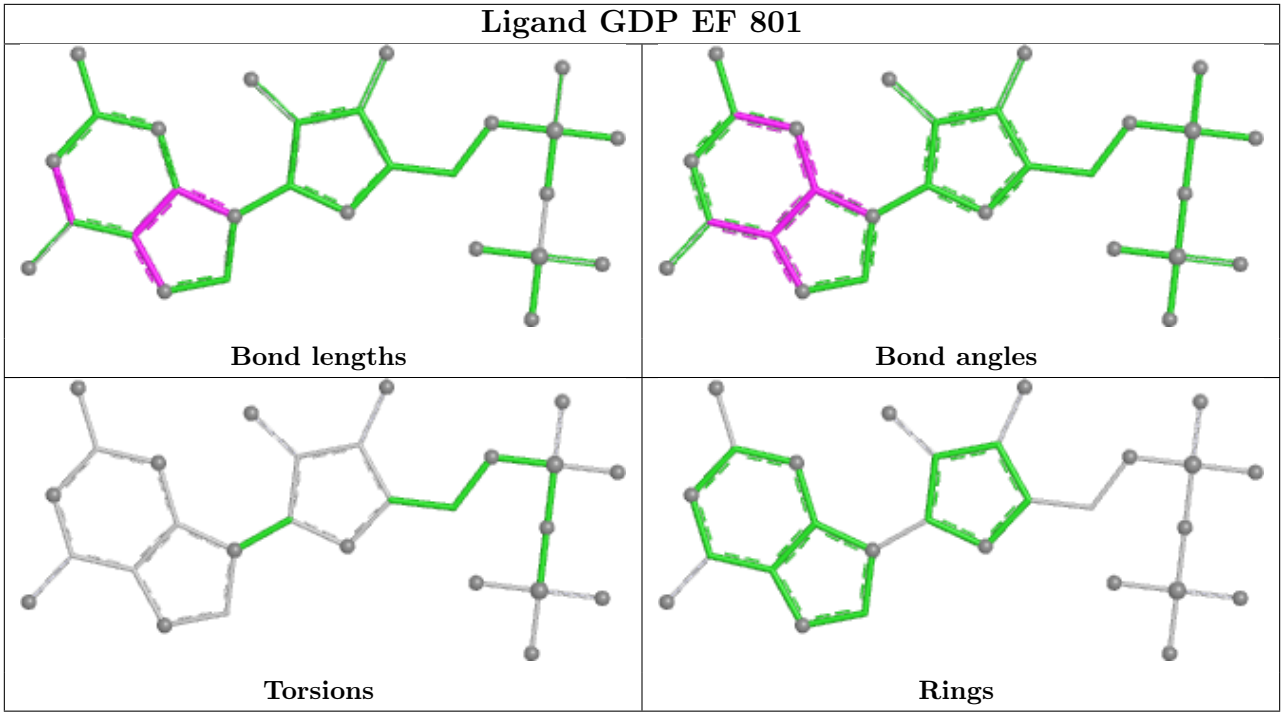
Mol	Chain	Res	Type	Atoms
66	Pt	3001	FME	N-CA-CB-CG
67	Pt	3002	PHE	C-CA-CB-CG
67	Pt	3002	PHE	CE2-CD2-CG-CD1
63	23	3010	SPD	C3-C4-C5-N6
66	Pt	3001	FME	O1-CN-N-CA
61	23	3002	PUT	C1-C2-C3-C4
66	Pt	3001	FME	CA-CB-CG-SD
66	Pt	3001	FME	C-CA-CB-CG
67	Pt	3002	PHE	N-CA-CB-CG
66	Pt	3001	FME	CB-CG-SD-CE
67	Pt	3002	PHE	CA-CB-CG-CD1
61	23	3005	PUT	C1-C2-C3-C4

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
67	Pt	3002	PHE	1	0
61	23	3004	PUT	1	0
63	23	3011	SPD	1	0
61	16	1601	PUT	1	0

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



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

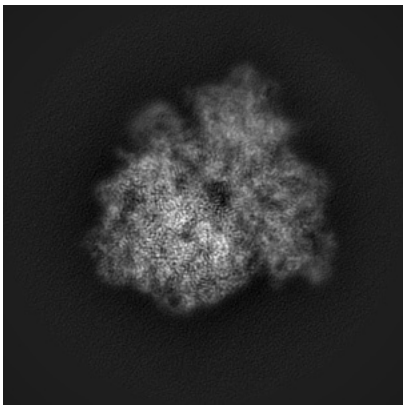
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-26486. These allow visual inspection of the internal detail of the map and identification of artifacts.

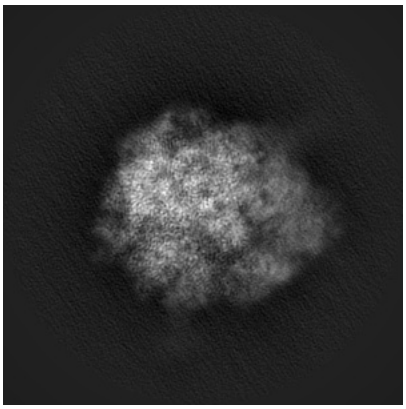
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

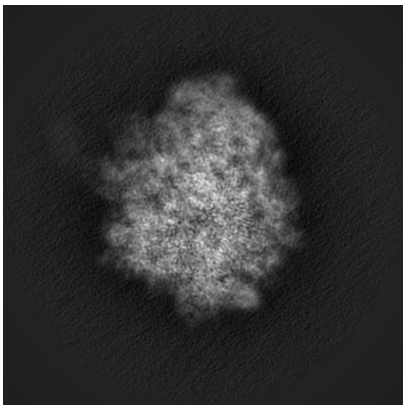
6.1.1 Primary map



X

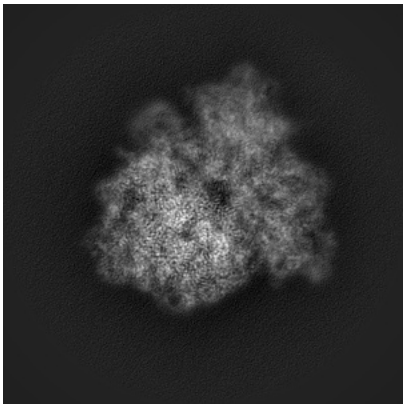


Y

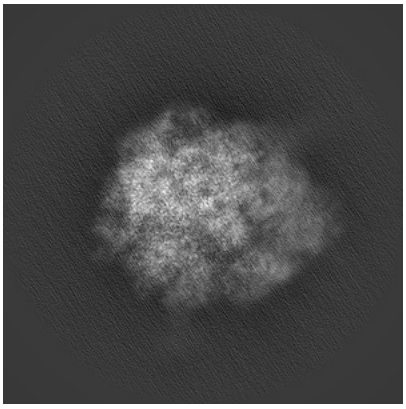


Z

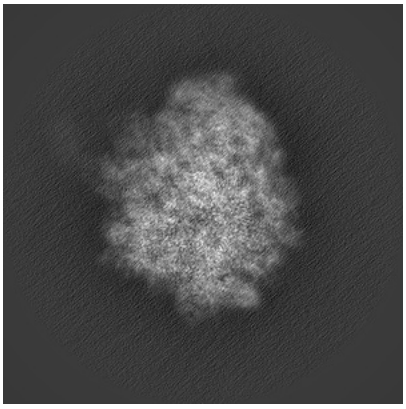
6.1.2 Raw map



X



Y

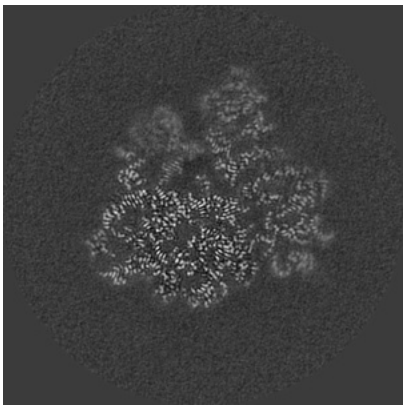


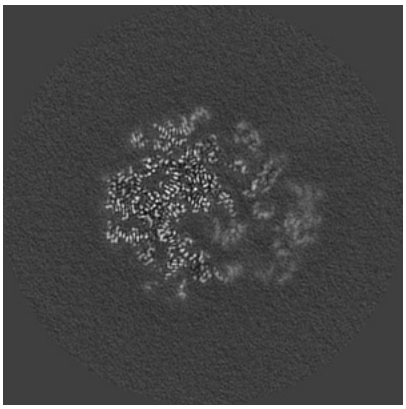
Z

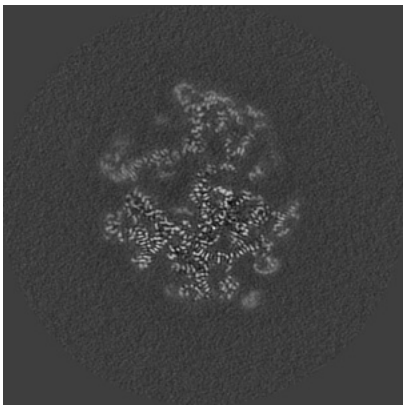
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

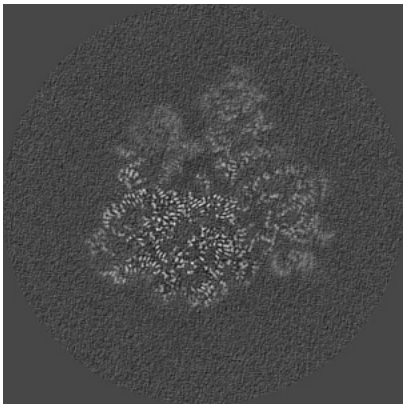
6.2.1 Primary map

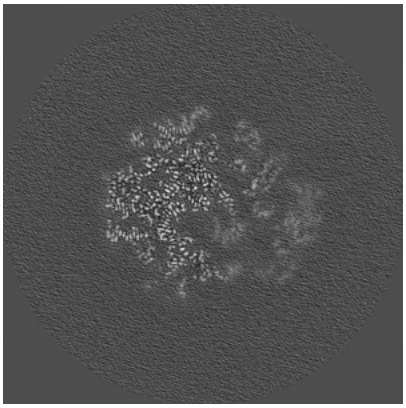

X Index: 190

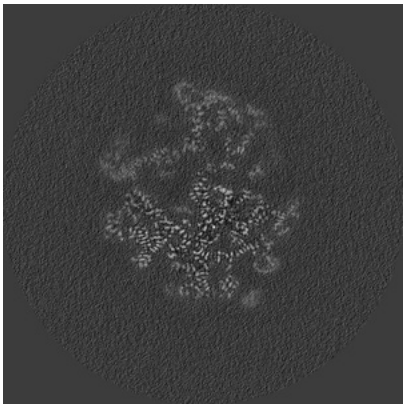

Y Index: 190


Z Index: 190

6.2.2 Raw map


X Index: 190

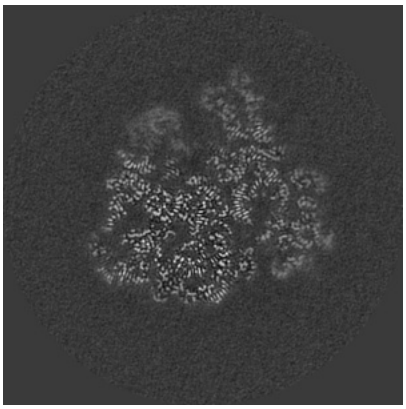

Y Index: 190


Z Index: 190

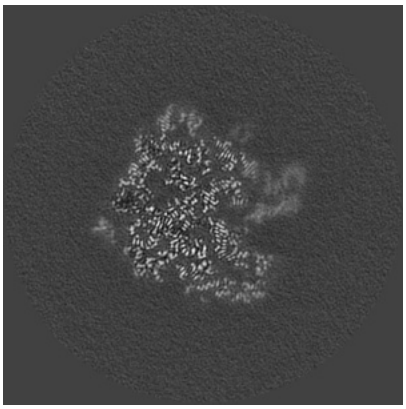
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

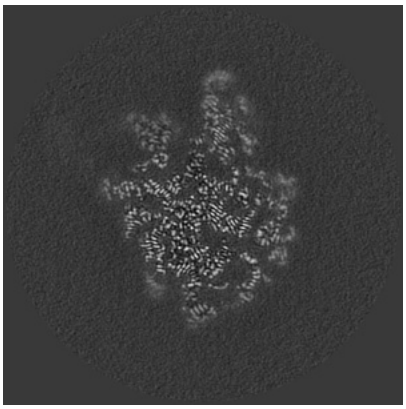
6.3.1 Primary map



X Index: 195

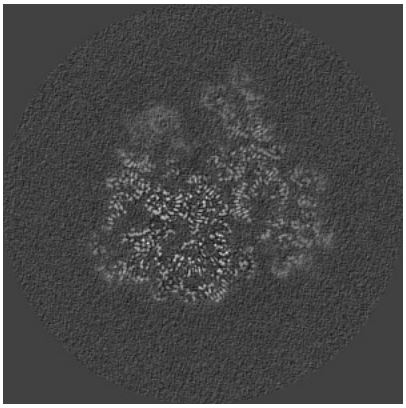


Y Index: 157

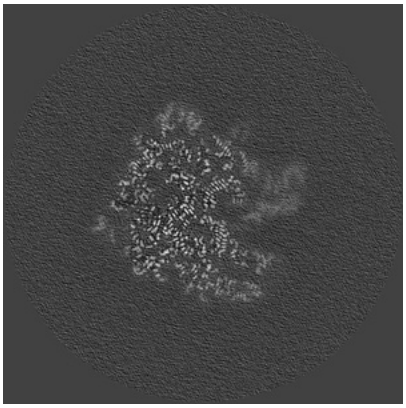


Z Index: 153

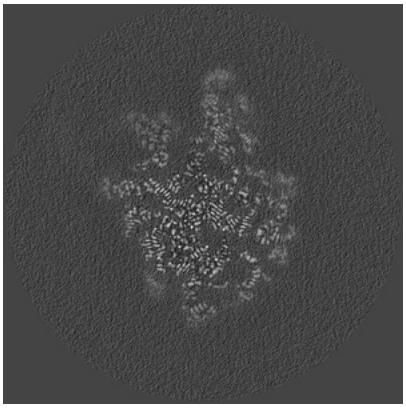
6.3.2 Raw map



X Index: 195



Y Index: 158

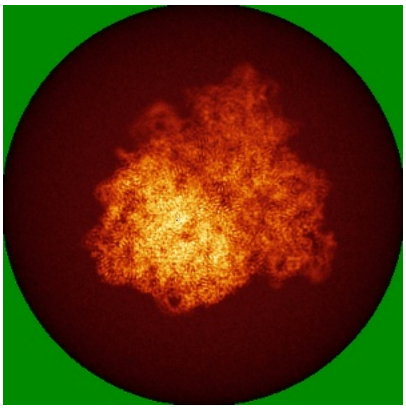


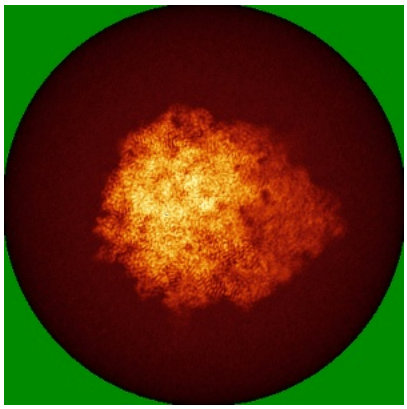
Z Index: 153

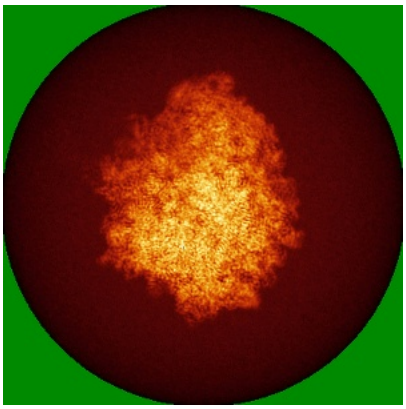
The images above show the largest variance slices of the map in three orthogonal directions.

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

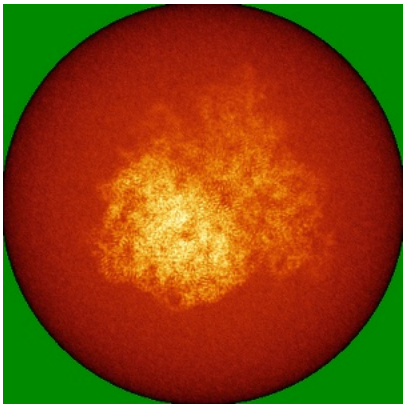
6.4.1 Primary map

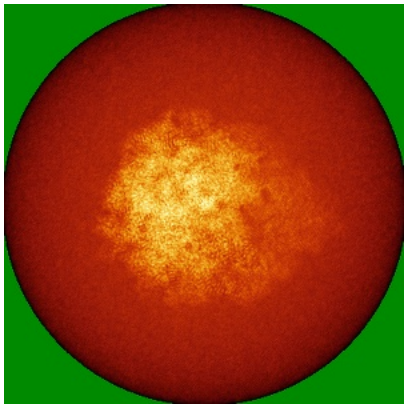

X

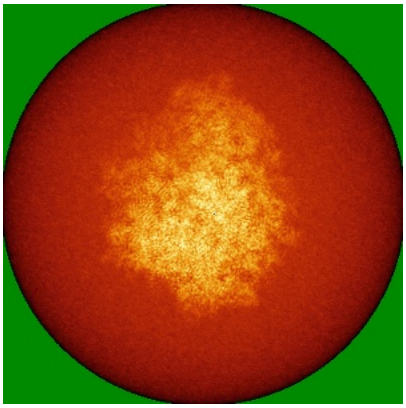

Y


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

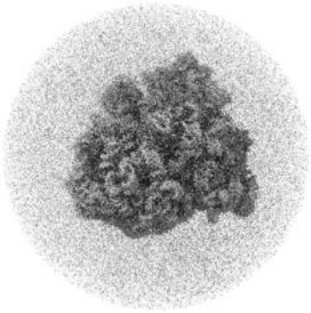
X

Y

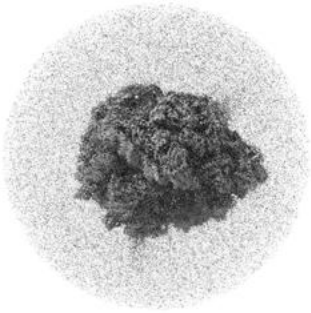
Z

The images above show the 3D surface view of the map at the recommended contour level 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

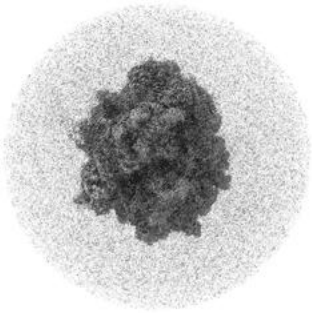
6.5.2 Raw map



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.

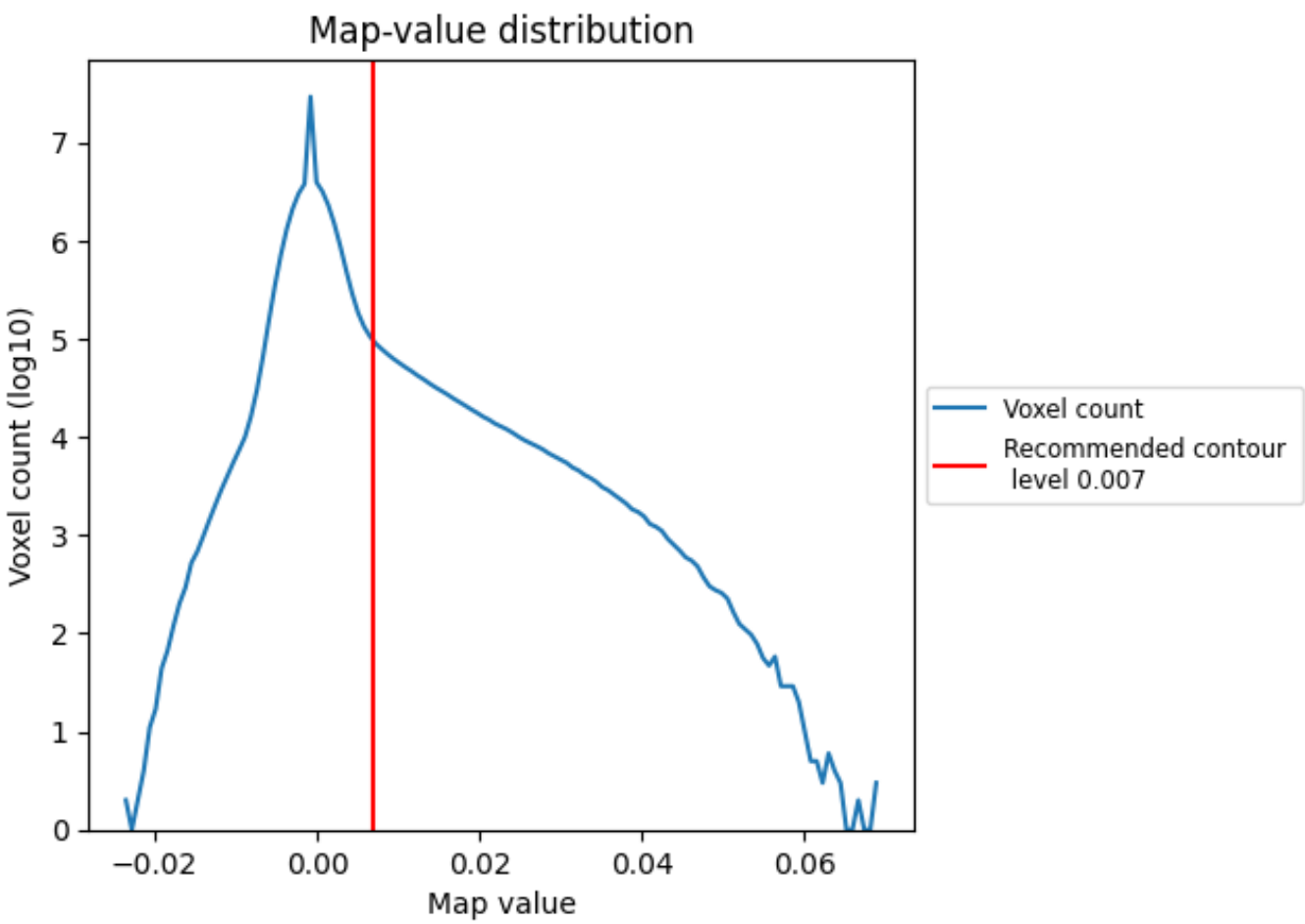
6.6 Mask visualisation (i)

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

7 Map analysis (i)

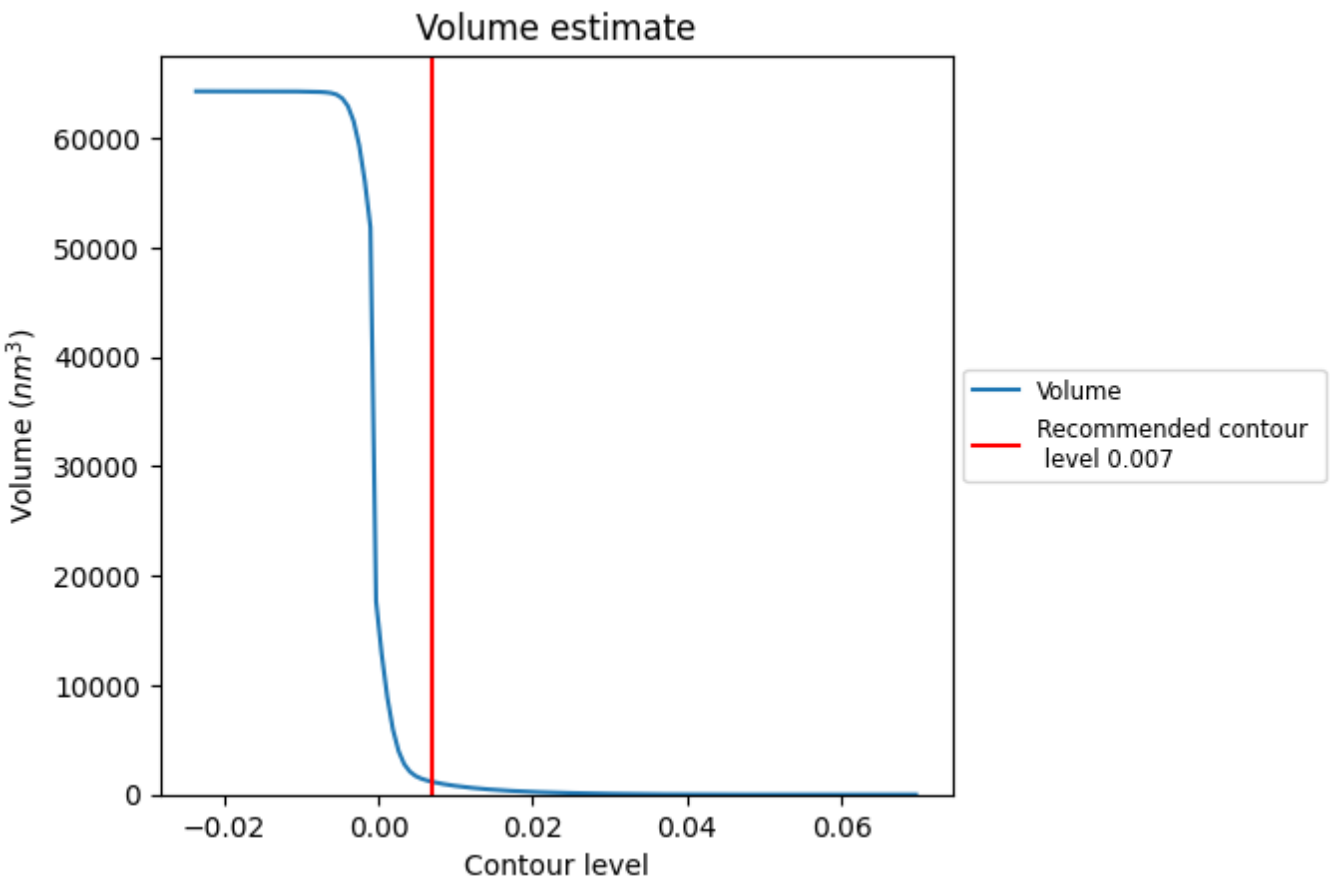
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

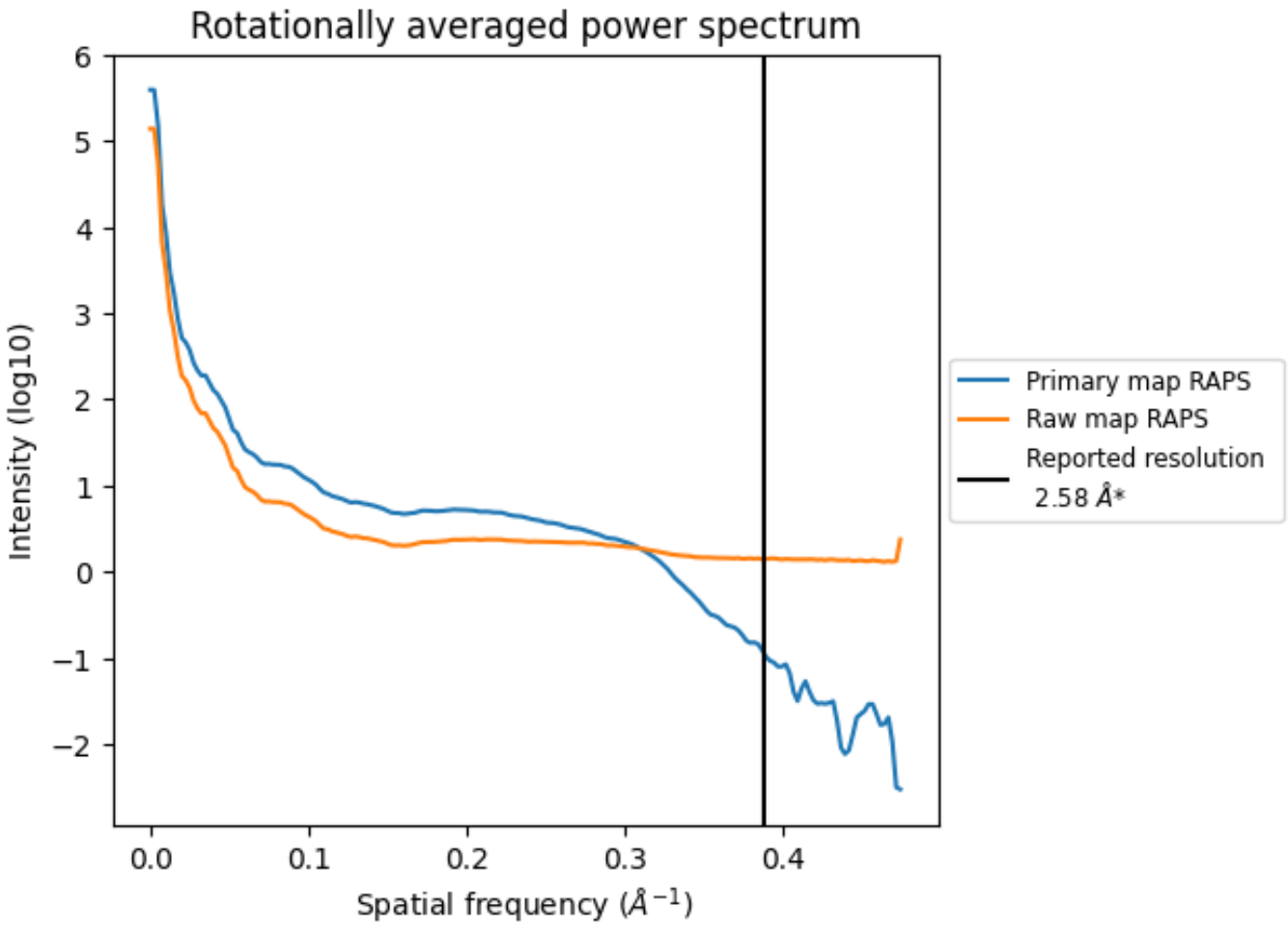
7.2 Volume estimate (i)



The volume at the recommended contour level is 1165 nm^3; this corresponds to an approximate mass of 1052 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)

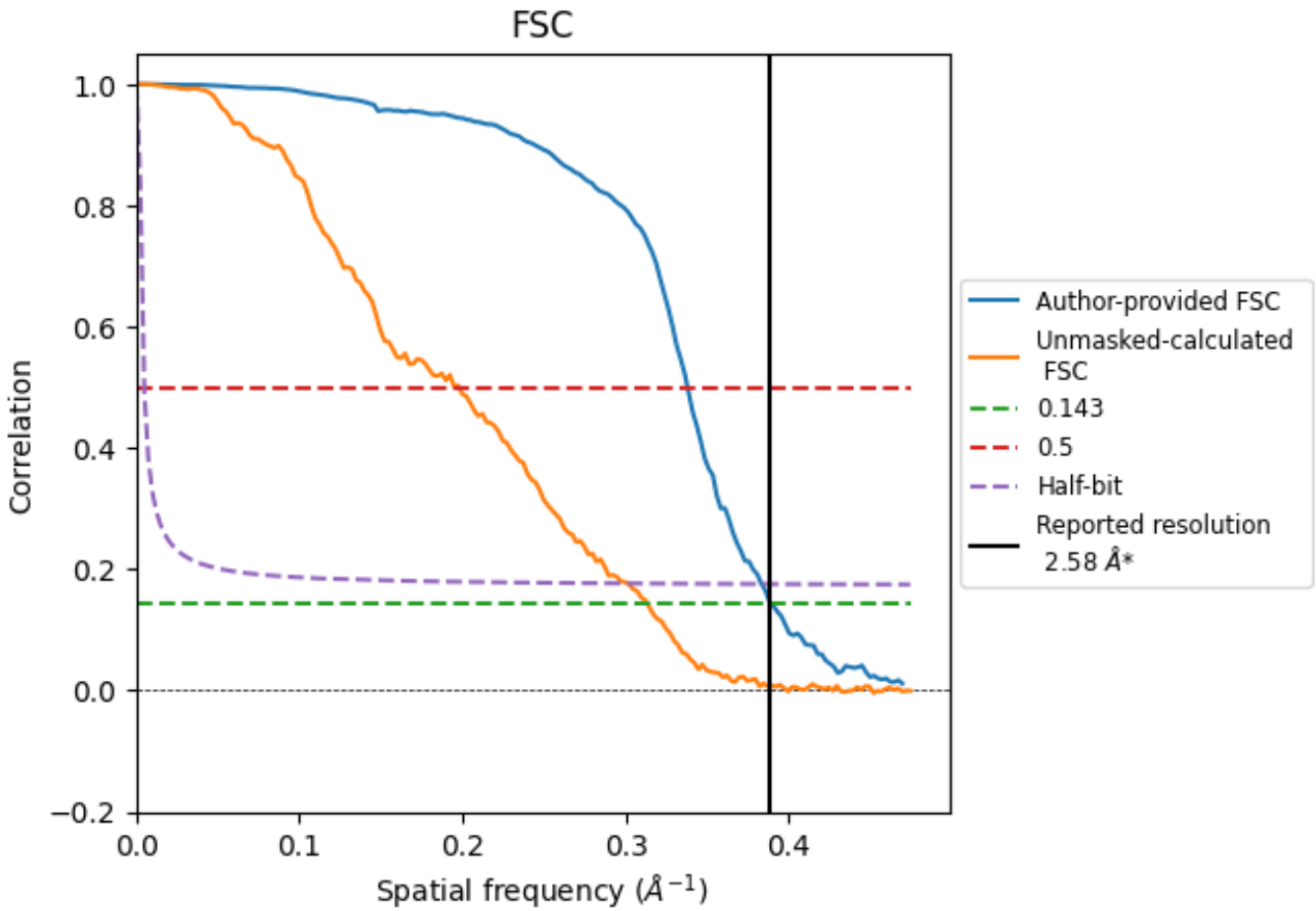


*Reported resolution corresponds to spatial frequency of 0.388 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.388 Å^{-1}

8.2 Resolution estimates (i)

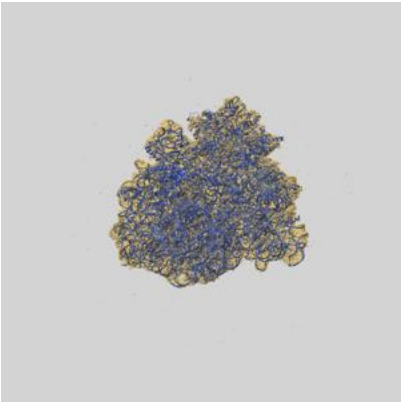
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.58	-	-
Author-provided FSC curve	2.57	2.96	2.61
Unmasked-calculated*	3.19	5.06	3.32

*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 3.19 differs from the reported value 2.58 by more than 10 %

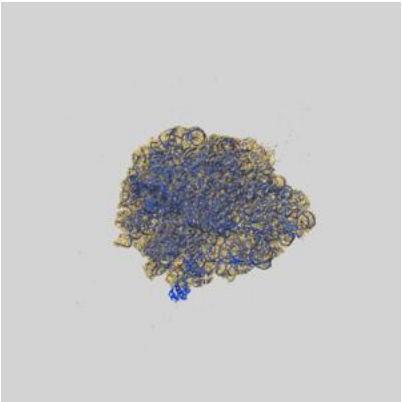
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-26486 and PDB model 7UG7. Per-residue inclusion information can be found in section 3 on page 19.

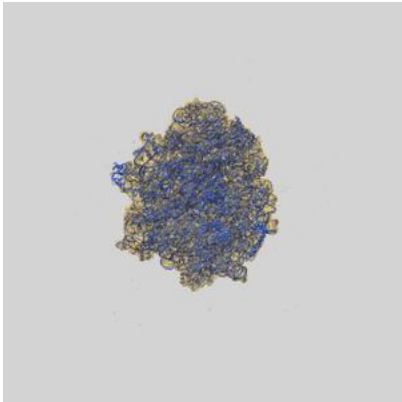
9.1 Map-model overlay (i)



X



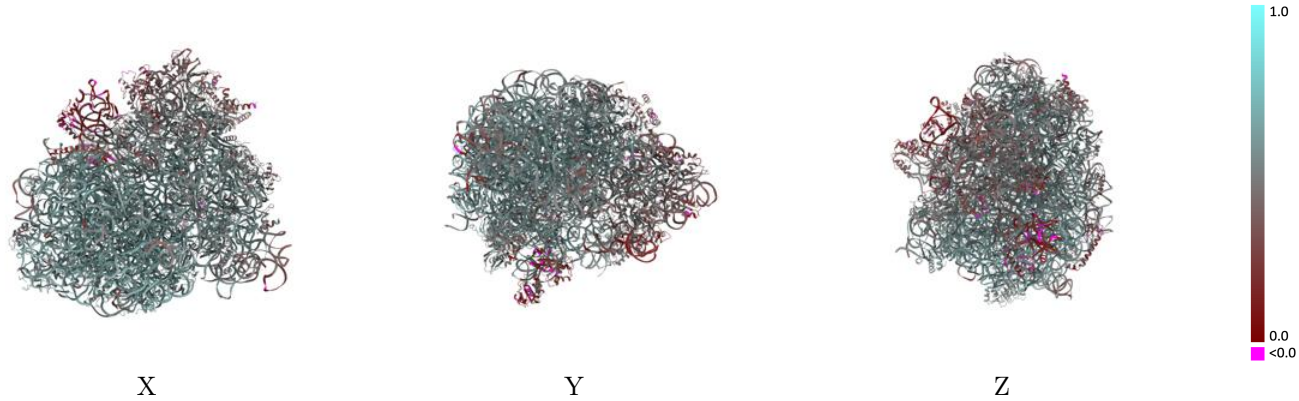
Y



Z

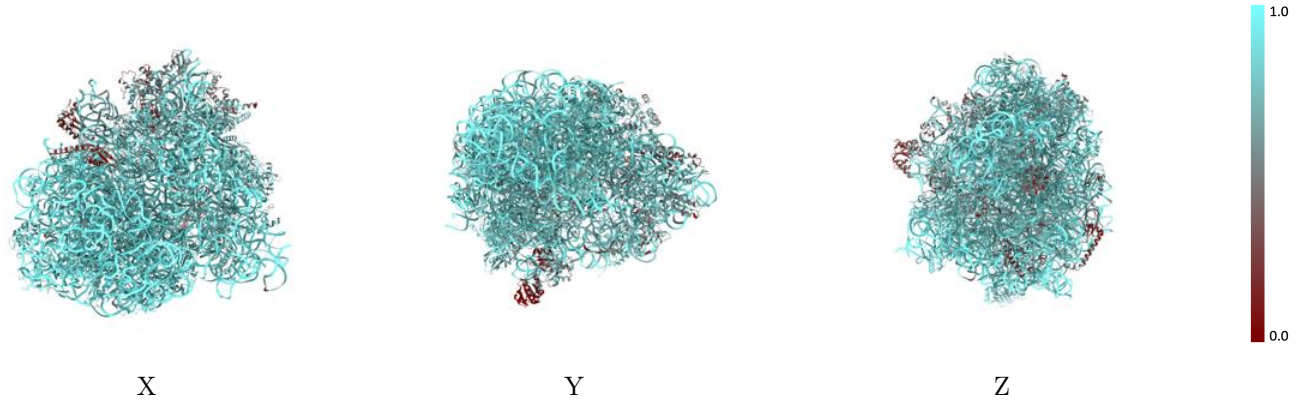
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



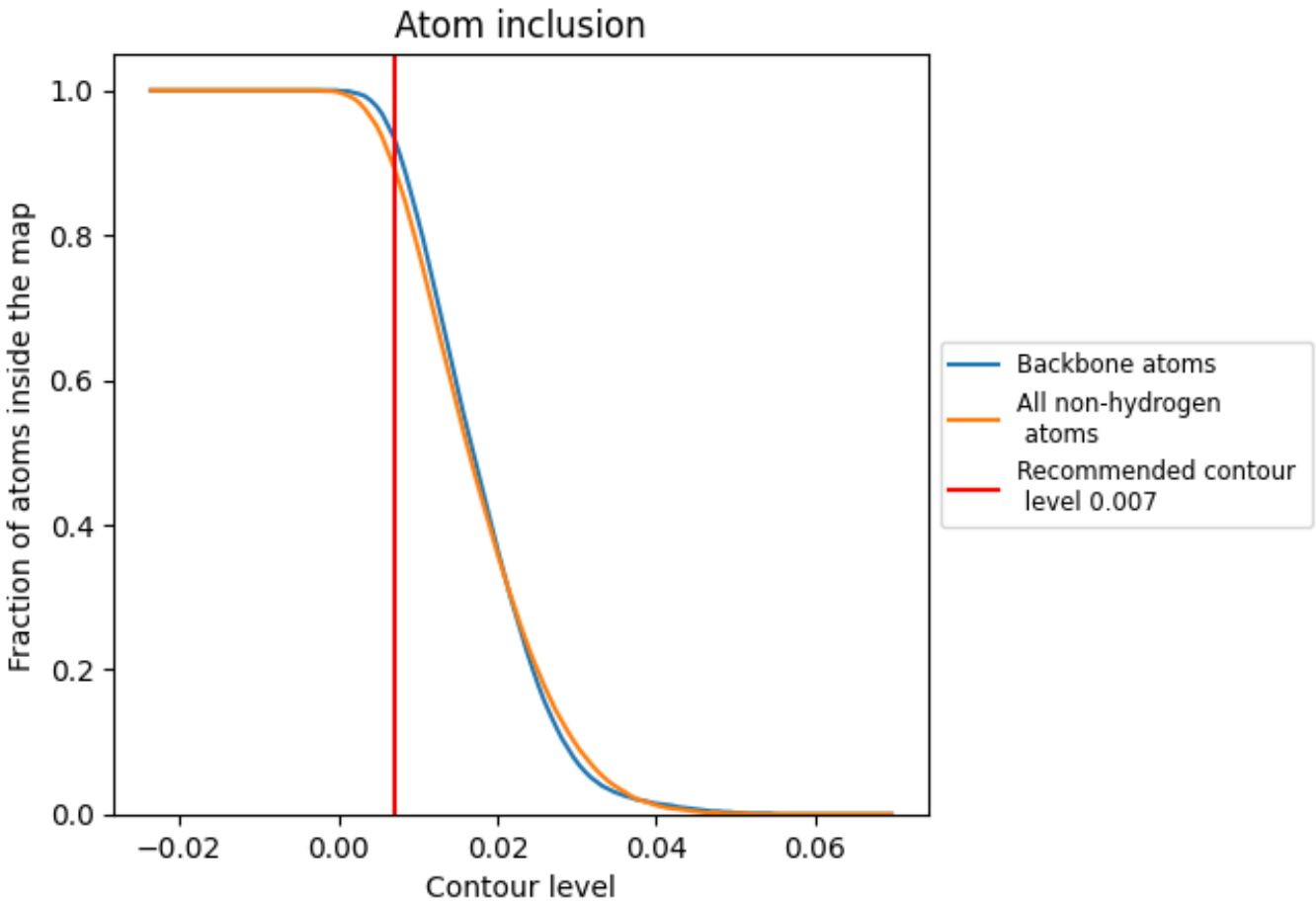
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.007).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8950	0.5360
16	0.9480	0.5160
23	0.9750	0.5870
5	0.9820	0.5590
B	0.8810	0.5290
Dt	0.8580	0.4840
EF	0.7300	0.4720
LA	0.2660	0.1840
LB	0.9300	0.6080
LC	0.9170	0.6030
LD	0.8930	0.5790
LE	0.7430	0.4420
LF	0.8430	0.5340
LI	0.3580	0.3090
LJ	0.2030	0.2680
LK	0.4100	0.2060
LM	0.9240	0.6070
LN	0.9050	0.6070
LO	0.8920	0.5760
LP	0.9200	0.6060
LQ	0.9590	0.6110
LR	0.8720	0.5370
LS	0.8730	0.5780
LT	0.9560	0.6110
LU	0.8810	0.5760
LV	0.9170	0.5980
LW	0.8660	0.5730
LX	0.8910	0.5620
LY	0.8640	0.5530
La	0.8930	0.6010
Lb	0.9200	0.5940
Lc	0.8590	0.5450
Ld	0.8880	0.5830
Le	0.5970	0.3510
Lf	0.8900	0.5880

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Lg	0.8580	0.5680
Lh	0.9440	0.6170
Li	0.9490	0.6180
Lj	0.8940	0.5900
Pt	0.8270	0.4850
SB	0.6330	0.4010
SC	0.6780	0.4370
SD	0.7750	0.4740
SE	0.8280	0.5140
SF	0.7120	0.4390
SG	0.4260	0.3060
SH	0.8060	0.5050
SI	0.6530	0.3970
SJ	0.5990	0.3670
SK	0.7890	0.4950
SL	0.8250	0.5600
SM	0.5660	0.3200
SN	0.7400	0.4080
SO	0.8350	0.5110
SP	0.7960	0.5000
SQ	0.8050	0.5320
SR	0.7860	0.4870
SS	0.6920	0.4060
ST	0.8180	0.5100
SU	0.7160	0.4650
mR	0.7570	0.4550