



Full wwPDB EM Validation Report ⓘ

Jun 22, 2026 – 10:21 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 ⓘ symbol.

The types of validation reports are described at

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

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

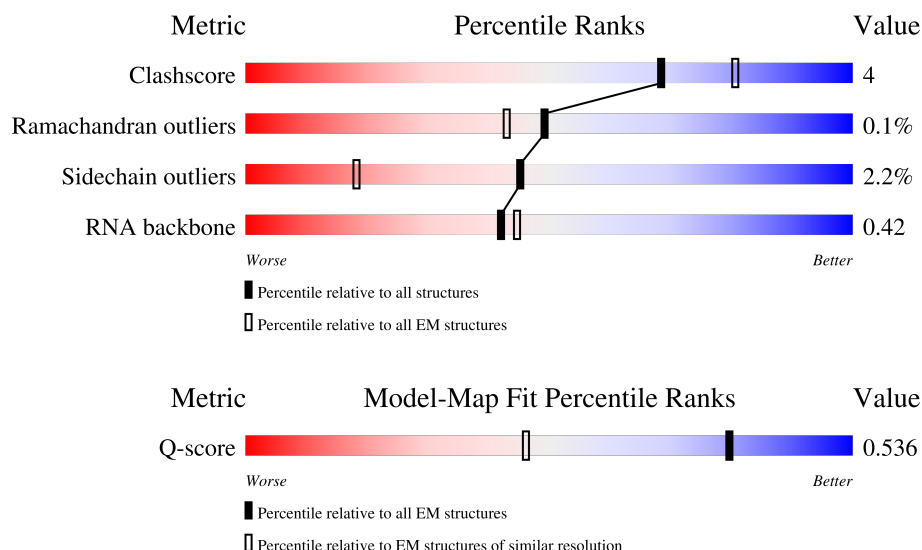
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 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.



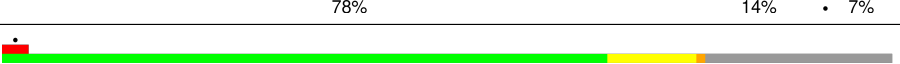
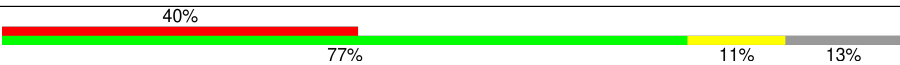
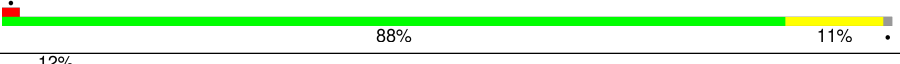
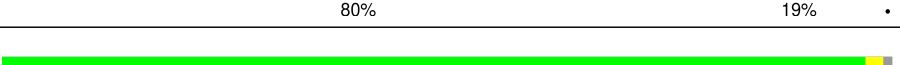
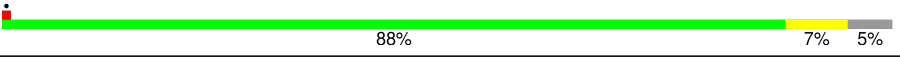
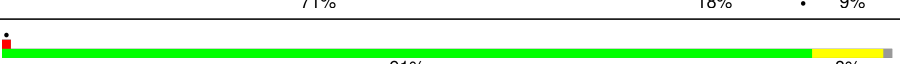
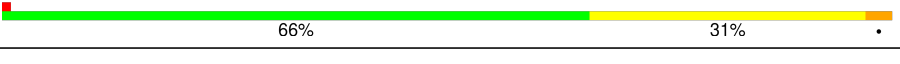
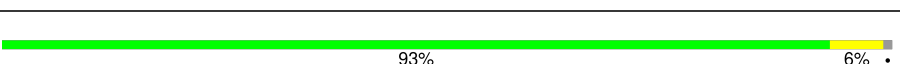
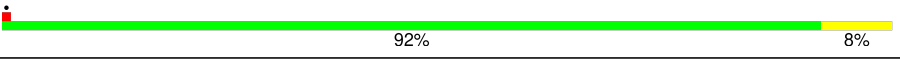
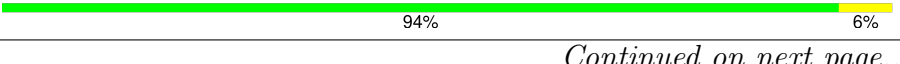
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7675 (2.08 - 3.08)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	16	1534	
2	SB	241	

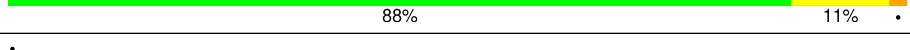
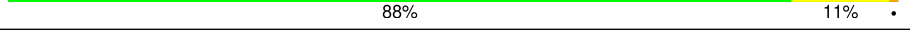
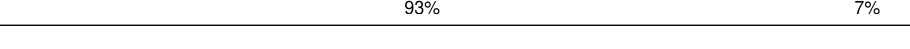
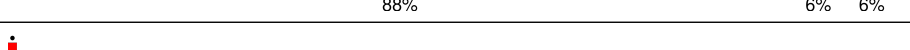
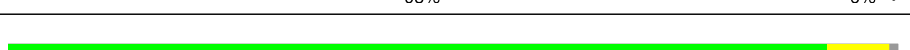
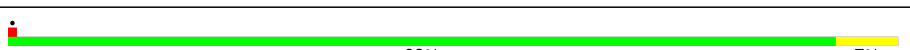
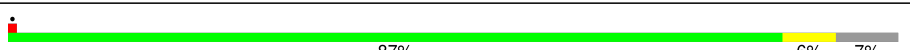
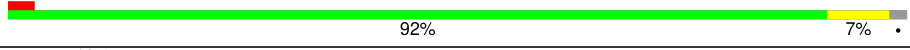
Continued on next page...

Continued from previous page...

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

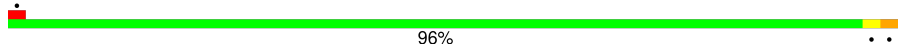
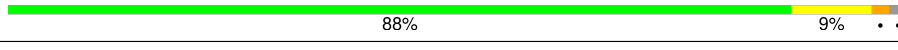
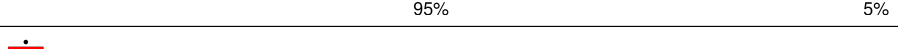
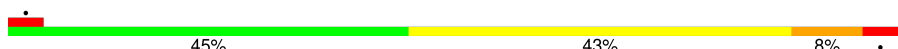
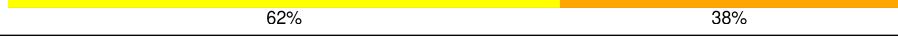
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
28	LE	179	
29	LF	177	
30	LI	149	
31	LJ	165	
32	LK	142	
33	LM	142	
34	LN	123	
35	LO	144	
36	LP	136	
37	LQ	127	
38	LR	117	
39	LS	115	
40	LT	118	
41	LU	103	
42	LV	110	
43	LW	100	
44	LX	104	
45	LY	94	
46	La	85	
47	Lb	78	
48	Lc	63	
49	Ld	59	
50	Le	70	
51	Lf	57	
52	Lg	55	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
53	Lh	46	
54	Li	65	
55	Lj	38	
56	EF	700	
57	Dt	77	
58	Pt	76	
59	mR	60	
60	B	8	

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
1	16	1514	Total	C	N	O	P	0	0
			32505	14503	5967	10521	1514		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 41 is a protein called Ribosomal protein L21.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 56 is a protein called Elongation factor G.

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

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

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

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

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

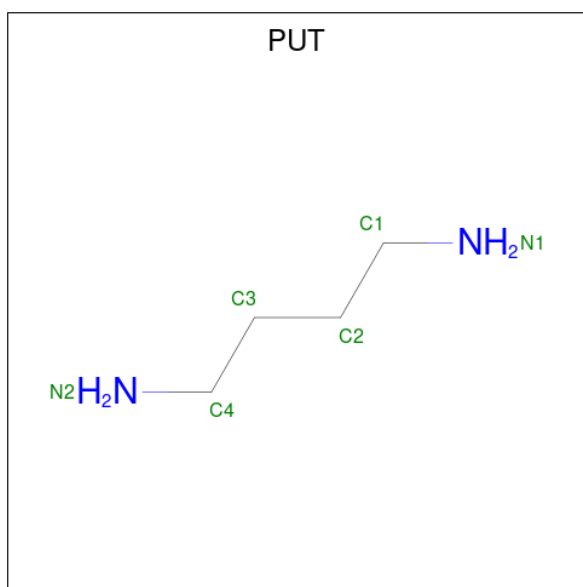
- Molecule 59 is a RNA chain called mRNA.

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

- Molecule 60 is a protein called Argyrin B.

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

- Molecule 61 is 1,4-DIAMINOBTUTANE (CCD ID: PUT) (formula: C₄H₁₂N₂).



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

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

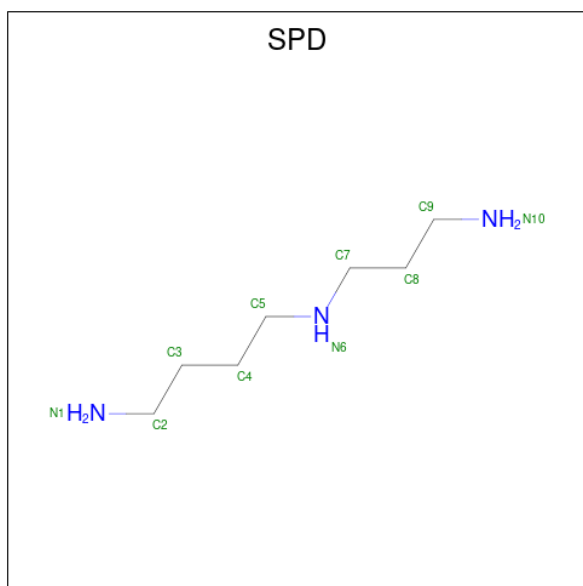
Mol	Chain	Residues	Atoms		AltConf
62	16	77	Total	Mg	0
			77	77	

Continued on next page...

Continued from previous page...

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

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

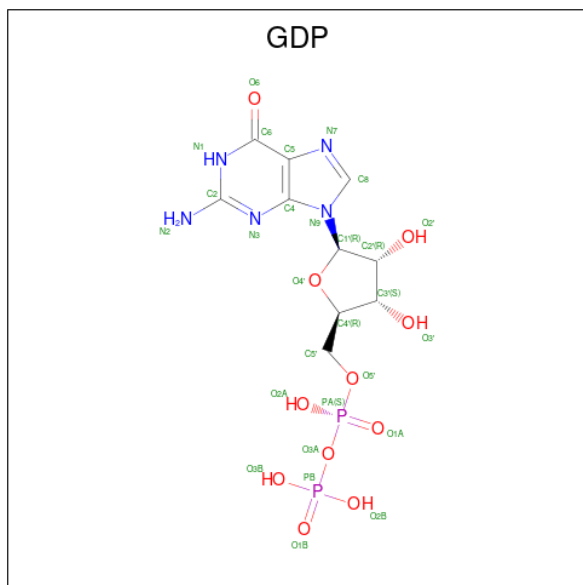


Mol	Chain	Residues	Atoms			AltConf
63	23	1	Total	C	N	0
			10	7	3	
63	23	1	Total	C	N	0
			10	7	3	

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

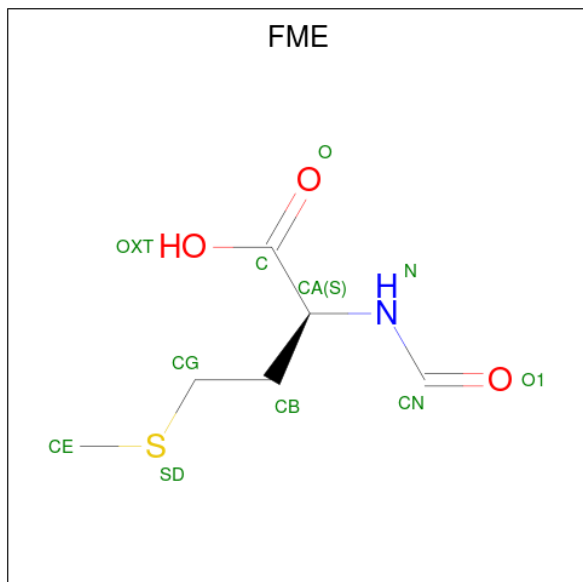
Mol	Chain	Residues	Atoms		AltConf
64	Le	1	Total	Zn	0
			1	1	
64	Lj	1	Total	Zn	0
			1	1	

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



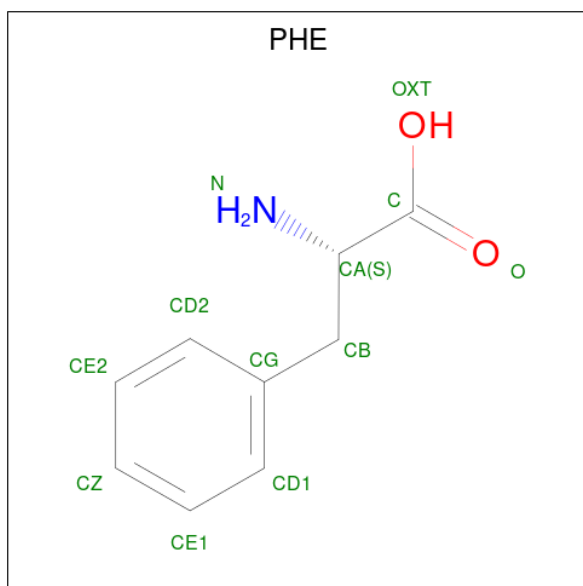
Mol	Chain	Residues	Atoms					AltConf
65	EF	1	Total	C	N	O	P	0
			28	10	5	11	2	

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

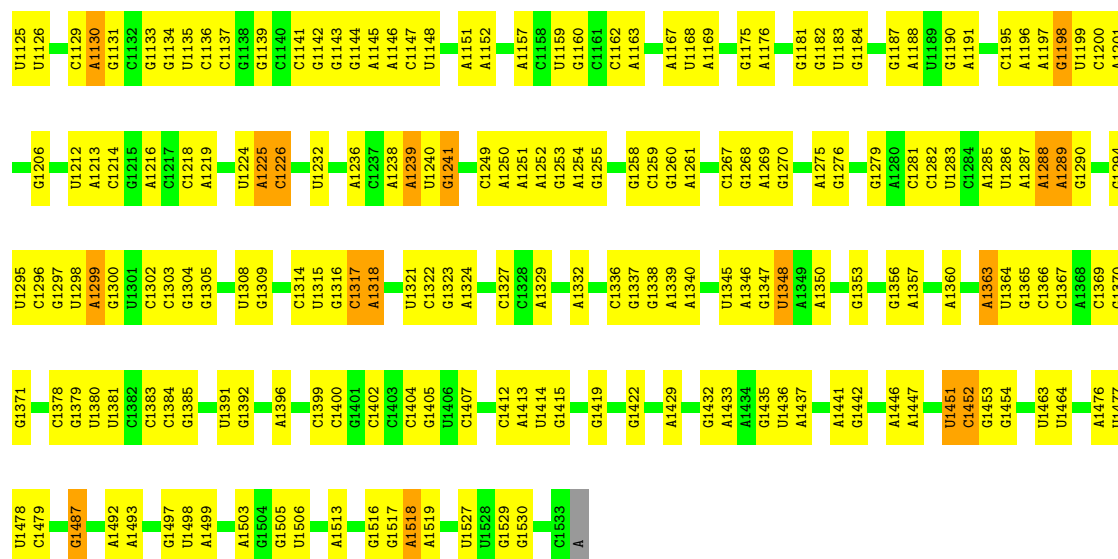


Mol	Chain	Residues	Atoms					AltConf
66	Pt	1	Total	C	N	O	S	0
			10	6	1	2	1	

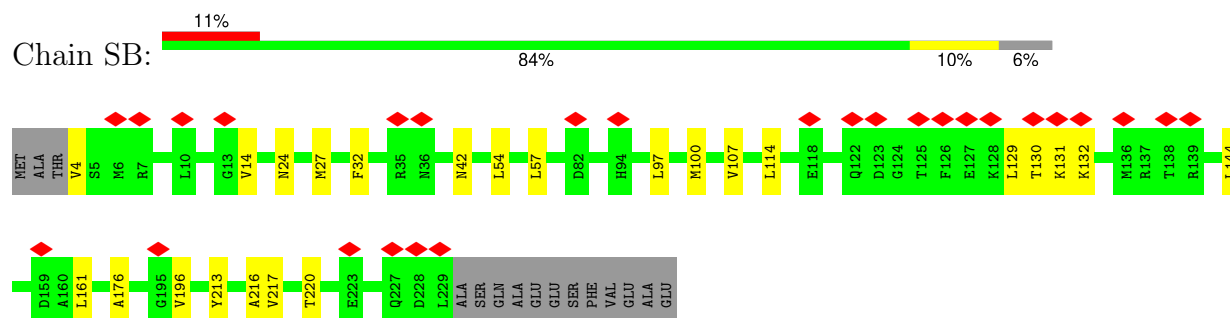
- Molecule 67 is PHENYLALANINE (CCD ID: PHE) (formula: $C_9H_{11}NO_2$).



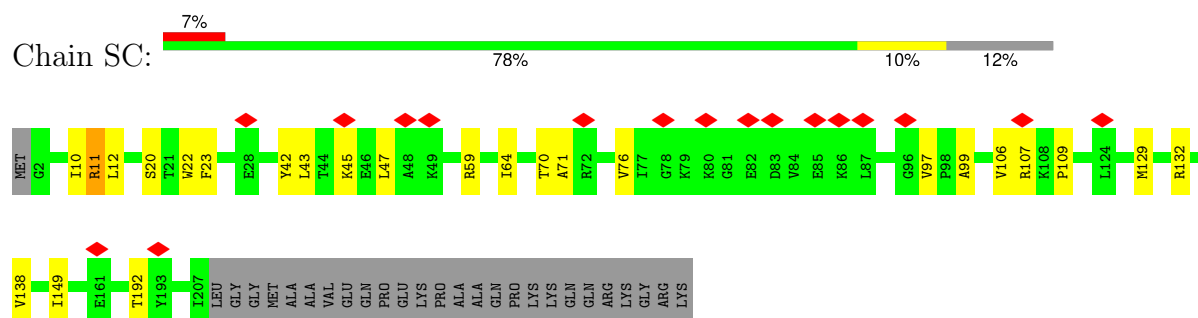
Mol	Chain	Residues	Atoms				AltConf
67	Pt	1	Total	C	N	O	0
			10	8	1	1	



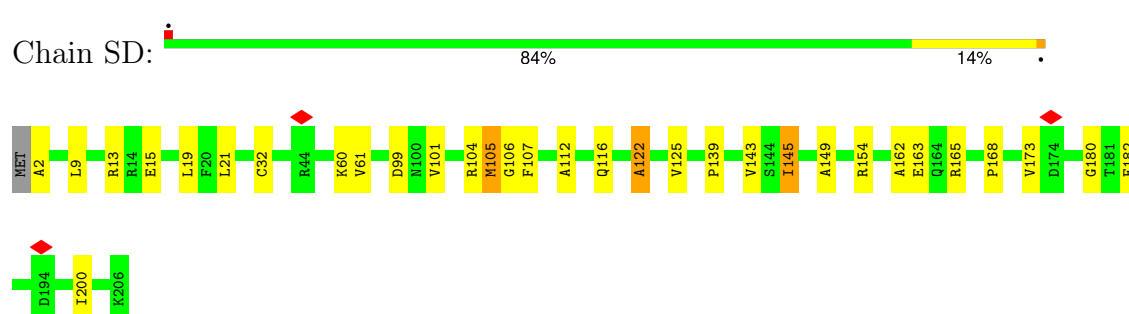
• Molecule 2: 30S ribosomal protein S2



• Molecule 3: 30S ribosomal protein S3



• Molecule 4: 30S ribosomal protein S4



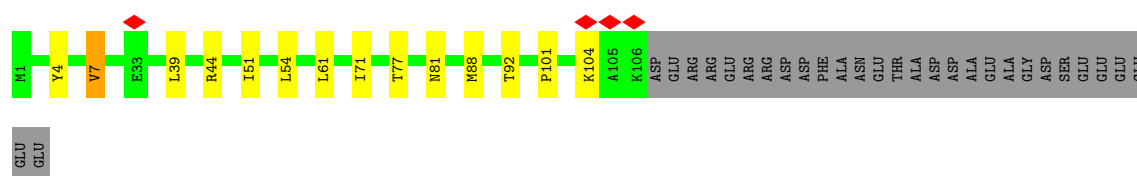
- Molecule 5: 30S ribosomal protein S5

Chain SE: 



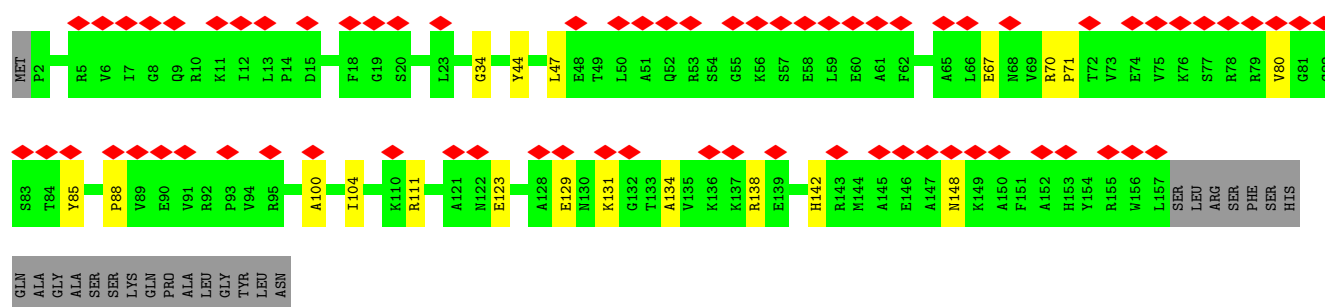
- Molecule 6: 30S ribosomal protein S6

Chain SF: 



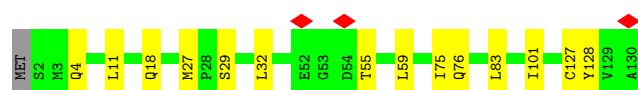
- Molecule 7: 30S ribosomal protein S7

Chain SG: 



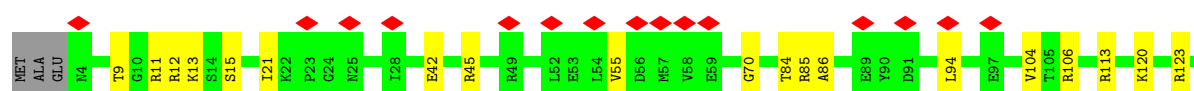
- Molecule 8: 30S ribosomal protein S8

Chain SH: 



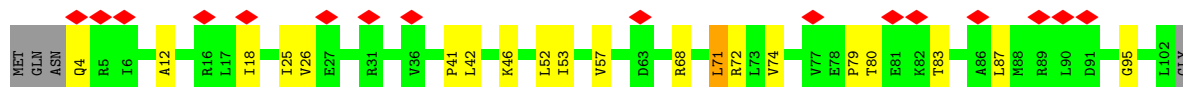
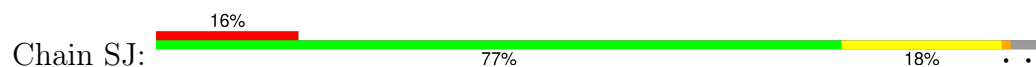
- Molecule 9: 30S ribosomal protein S9

Chain SI: 

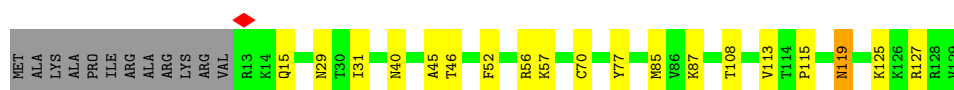
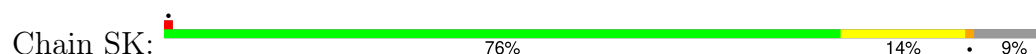




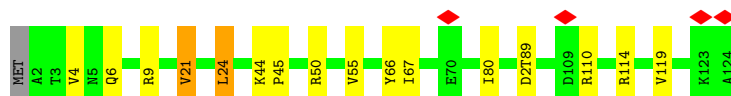
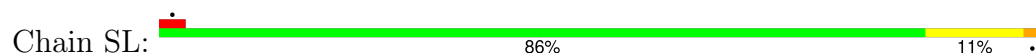
- Molecule 10: 30S ribosomal protein S10



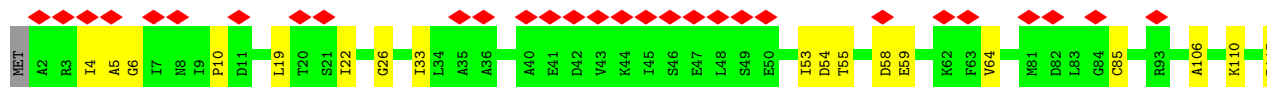
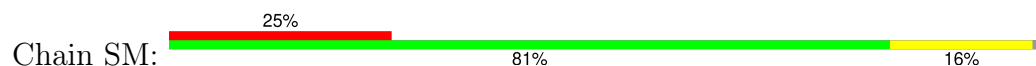
- Molecule 11: 30S ribosomal protein S11



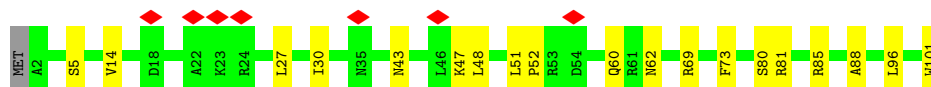
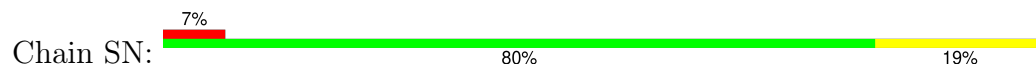
- Molecule 12: 30S ribosomal protein S12



- Molecule 13: 30S ribosomal protein S13

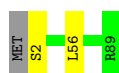


- Molecule 14: 30S ribosomal protein S14

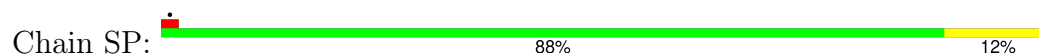


- Molecule 15: 30S ribosomal protein S15

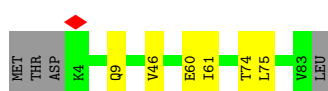
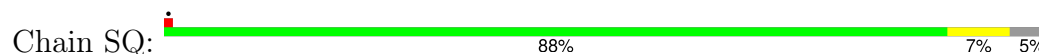




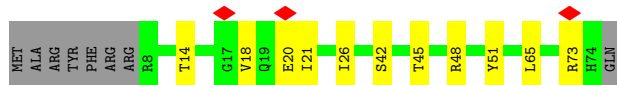
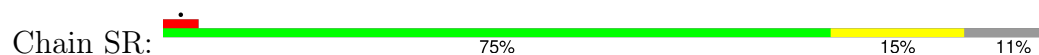
- Molecule 16: 30S ribosomal protein S16



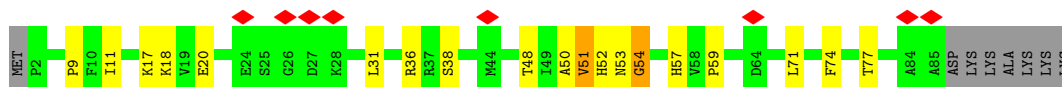
- Molecule 17: 30S ribosomal protein S17



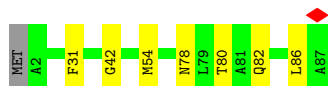
- Molecule 18: 30S ribosomal protein S18



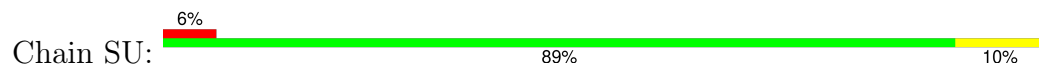
- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein S21

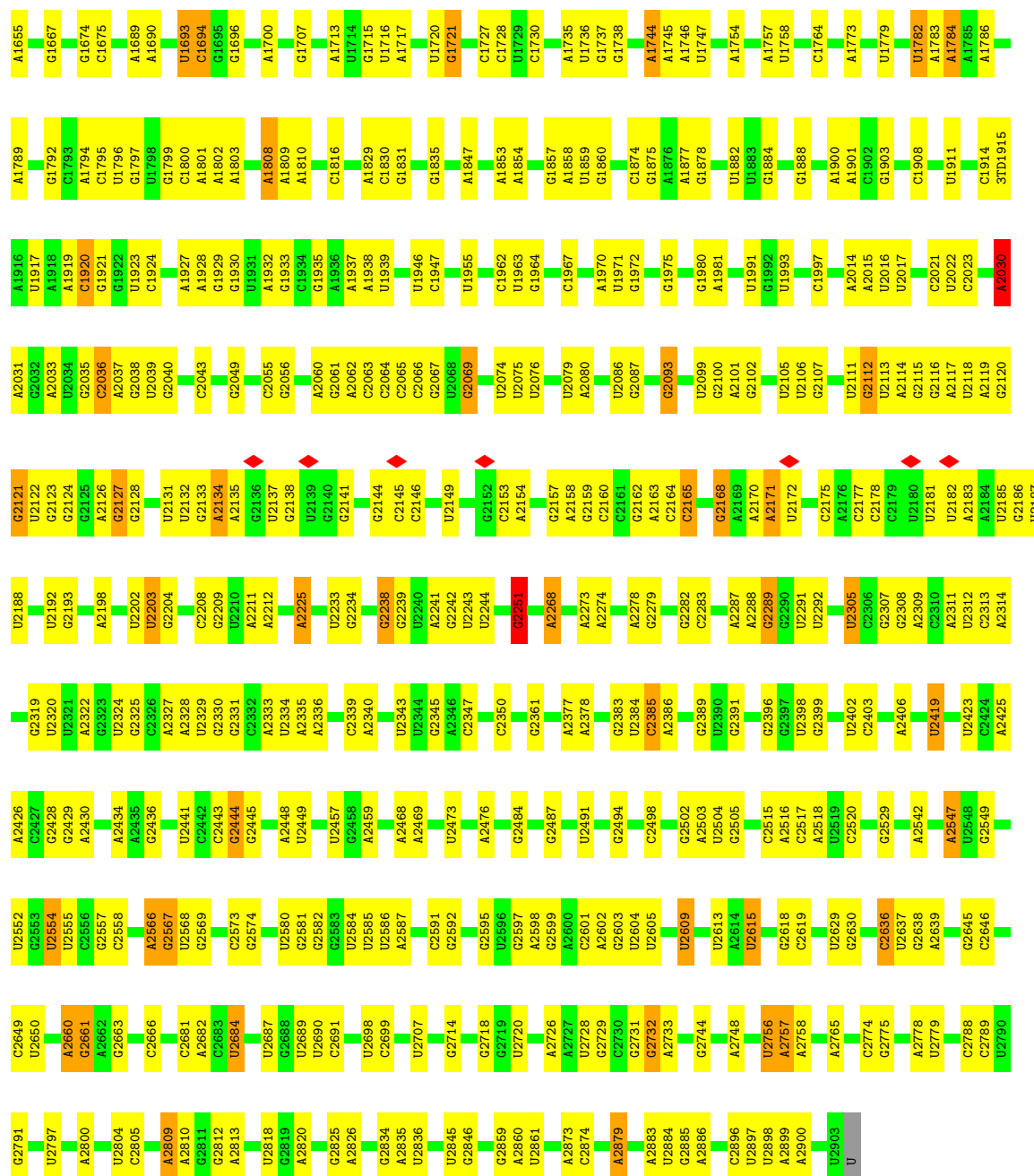


- Molecule 22: 23S rRNA

Chain 23:

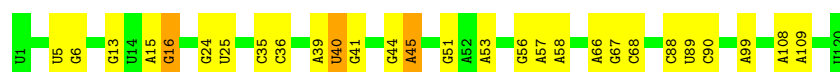


G1524	G1529	U1534	A1535	G1537	G1538	U1539	G1540	A1544	A1545	A1548	A1549	C1558	A1566	G1567	G1568	A1569	U1578	A1579	A1580	A1583	U1584	C1605	C1606	C1607	A1608	A1609	A1610	C1615	A1616	C1617	A1618	G1619	A1634	A1635	U1636	A1637	G1645	C1646	U1647	U1648	G1649	A1650	G1651	A1654									
G1407	A1413	G1416	C1417	A1420	G1421	G1425	G1426	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	A1635	U1636	A1637	G1645	C1646	U1647	U1648	G1649	A1650	G1651	A1654							
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														
U1148	A1156	C1170	G1171	C1172	U1174	A1175	U1176	G1177	C1178	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										
U1033	A911	C912	U913	G914	A917	A927	U931	U932	A933	U934	A941	C946	A947	C948	U946	U947	U948	U949	U950	C951	U952	G956	G957	G958	G959	C965	A866	G969	U870	U871	U872	A877	A878	G879	G880	C881	C885	A886	U887	C888	C889	C990	A991	A992	C993	U894	U895	A896	U906	C907	C908	A909	A910
U1033	A911	C912	U913	G914	A917	A927	U931	U932	A933	U934	A941	C946	A947	C948	U946	U947	U948	U949	U950	C951	U952	G956	G957	G958	G959	C965	A866	G969	U870	U871	U872	A877	A878	G879	G880	C881	C885	A886	U887	C888	C889	C990	A991	A992	C993	U894	U895	A896	U906	C907	C908	A909	A910
U1033	A911	C912	U913	G914	A917	A927	U931	U932	A933	U934	A941	C946	A947	C948	U946	U947	U948	U949	U950	C951	U952	G956	G957	G958	G959	C965	A866	G969	U870	U871	U872	A877	A878	G879	G880	C881	C885	A886	U887	C888	C889	C990	A991	A992	C993	U894	U895	A896	U906	C907	C908	A909	A910
U1033	A911	C912	U913	G914	A917	A927	U931	U932	A933	U934	A941	C946	A947	C948	U946	U947	U948	U949	U950	C951	U952	G956	G957	G958	G959	C965	A866	G969	U870	U871	U872	A877	A878	G879	G880	C881	C885	A886	U887	C888	C889	C990	A991	A992	C993	U894	U895	A896	U906	C907	C908	A909	A910
U1033	A911	C912	U913	G914	A917	A927	U931	U932	A933	U934	A941	C946	A947	C948	U946	U947	U948	U949	U950	C951	U952	G956	G957	G958	G959	C965	A866	G969	U870	U871	U872	A877	A878	G879	G880	C881	C885	A886	U887	C888	C889	C990	A991	A992	C993	U894	U895	A896	U906	C907	C908	A909	A910
U1033	A911	C912	U913	G914	A917	A927	U931	U932	A933	U934	A941	C946	A947	C948	U946	U947	U948	U949	U950	C951	U952	G956	G957	G958	G959	C965	A866	G969	U870	U871	U872	A877	A878	G879	G880	C881	C885	A886	U887	C888	C889	C990	A991	A992	C993	U894	U895	A896	U906	C907	C908	A909	A910
U1033	A911	C912	U913	G914	A917	A927	U931	U932	A933	U934	A941	C946	A947	C948	U946	U947	U948	U949	U950	C951	U952	G956	G957	G958	G959	C965	A866	G969	U870	U871	U872	A877	A878	G879	G880	C881	C885	A886	U887	C888	C889	C990	A991	A992	C993	U894	U895	A896	U906	C907	C908	A909	A910
U1033	A911	C912	U913	G914	A917	A927	U931	U932	A933	U934	A941	C946	A947	C948	U946	U947	U948	U949	U950	C951	U952	G956	G957	G958	G959	C965	A866	G969	U870	U871	U872	A877	A878	G879	G880	C881	C885	A886	U887	C888	C889	C990	A991	A992	C993	U894	U895	A896	U906	C907	C908	A909	A910
U1033	A911	C912	U913	G914	A917	A927	U931	U932	A933	U934	A941	C946	A947	C948	U946	U947	U948	U949	U950	C951	U952	G956	G957	G958	G959	C965	A866	G969	U870	U871	U872	A877	A878	G879	G880	C881	C885	A886	U887	C888	C889	C990	A991	A992	C993	U894	U895	A896	U906	C907	C908	A909	A910
U1033	A911	C912	U913	G914	A917	A927	U931	U932	A933	U934	A941	C946	A947	C948	U946	U947	U948	U949	U950	C951	U952	G956	G957	G958	G959	C965	A866	G969	U870	U871	U872	A877	A878	G879	G880	C881	C885	A886	U887	C888	C889	C990	A991	A992	C993	U894	U895	A896	U906	C907	C908	A909	A910
U1033	A911	C912	U913	G914	A917	A927	U931	U932	A933	U934	A941	C946	A947	C948	U946	U947	U948	U949	U950	C951	U952	G956	G957	G958	G959	C965	A866	G969	U870	U871	U872	A877	A878	G879	G880	C881	C885	A886	U887	C888	C889	C990	A991	A992	C993	U894	U895	A896	U906	C907	C908	A909	A910
U1033	A911	C912	U913	G914	A917	A927	U931	U932	A933	U934	A941	C946	A947	C948	U946	U947	U948	U949	U950	C951	U952	G956	G957	G958	G959	C965	A866	G969	U870	U871	U872	A877	A878	G879	G880	C881	C885	A886	U887	C888	C889	C990	A991	A992	C993	U894	U895	A896	U906	C907	C908	A909	A910
U1033	A911	C912	U913	G914	A917	A927	U931	U932	A933	U934	A941	C946	A947	C948	U946	U947	U948	U949	U950	C951	U952	G956	G957	G958	G959	C965	A866	G969	U870	U871	U872	A877	A878	G879	G880	C881	C885	A886	U887	C888	C889	C990	A991	A992	C993	U894	U895	A896	U906	C907	C908	A909	A910
U1033	A911	C912	U913	G914	A917	A927	U931	U932	A933	U934	A941	C946	A947	C948	U946	U947	U948	U949	U950	C951	U952	G956	G957	G958	G959	C965	A866	G969	U870	U871	U872	A877	A878	G879	G880	C881	C885	A886	U887	C888	C889	C990	A991	A992	C993	U894	U895	A896	U906	C907	C908	A909	A910
U1033	A911	C912	U913	G914	A917	A927	U931	U932	A933	U934	A941	C946	A947	C948	U946	U947	U948	U949	U950	C951	U952	G956	G957	G958	G959	C965	A866	G969	U870	U871	U872	A877	A878	G879	G880	C881	C885	A886	U887	C888	C889	C990	A991	A992	C993	U894	U895	A896	U906	C907	C908	A909	A910
U1033	A911	C912	U913	G914	A917	A927	U931	U932	A933	U934	A941	C946	A947	C948	U946	U947	U948	U949	U950	C951	U952	G956	G957	G958	G959	C965	A866	G969	U870	U871	U872	A877	A878	G879	G880	C881	C885	A886	U887	C888	C889	C990	A991	A992	C993	U894	U895	A896	U906	C907	C908	A909	A910
U1033	A911	C912	U913	G914	A917	A927	U931	U932	A933	U934	A941	C946	A947	C948	U946	U947	U948	U949	U950	C951	U952	G956	G957	G958	G959	C965	A866	G969	U870	U871	U872	A877	A878	G879	G880	C881	C885	A886	U887	C888	C889	C990	A991	A992	C993	U894	U895	A896	U906	C907	C908	A909	A910
U1033	A911	C912	U913	G914	A917	A927	U931	U932	A933	U934	A941	C946	A947	C948	U946	U947	U948	U949	U950	C951	U952	G956	G957	G958	G959	C965	A866	G969	U870	U871	U872	A877	A878	G879	G880	C881	C885	A886	U887	C888	C889	C990	A991	A992	C993	U894	U895	A896	U906	C907	C908	A909	A910
U1033	A911	C912	U913	G914	A917	A927	U931	U932	A933	U934	A941	C946	A947	C948	U946	U947	U948	U949	U950	C951	U952	G956	G957	G958	G959	C965	A866	G969	U870	U871	U872	A877	A878	G879	G880	C881	C885	A886	U887	C888	C889	C990	A991	A992	C993	U894	U895	A896	U906	C907	C908	A909	A910
U1033	A911	C912	U913	G914	A917	A927	U931	U932	A933	U934	A941	C946	A947	C948	U946	U947	U948	U949	U950	C951	U952	G956	G957	G958	G959	C965	A866	G969	U870	U871	U872	A877	A878	G879	G880	C881	C885	A886	U887	C888	C889	C990	A991	A992	C993	U894	U895	A896	U906	C907	C908	A909	A910
U1033	A911	C912	U913	G914	A917	A927	U931	U932	A933	U934	A941	C946	A947	C948	U946	U947	U948	U949	U950	C951	U952	G956	G957	G958	G959	C965	A866	G969	U870	U871	U872	A877	A878	G879	G880	C881	C885	A886	U887	C888	C889	C990	A991	A992	C993	U894	U895	A896	U906	C907	C908	A909	A910
U1033	A911	C912	U913	G914	A917	A927	U931	U932	A933	U934	A941	C946	A947	C948	U946	U947	U948	U949	U950	C951	U952	G956	G957	G958	G959	C965	A866	G969	U870	U871	U872	A877	A878	G879	G880	C881	C885	A886	U887	C888	C889	C990	A991	A992	C993	U894	U895	A896	U906	C907	C908	A909	A910
U1033	A911	C912	U913	G914	A917	A927	U931	U932	A933	U934	A941	C946	A947	C948	U946	U947	U948	U949	U950	C951	U952	G956	G957	G958	G959	C965	A866	G969	U870	U871	U872	A877	A878	G879	G880	C881	C885	A886	U887	C888	C889	C990	A991	A992	C993	U894	U895	A896	U906	C907	C908	A909	A910
U1033	A911	C912	U913	G914	A917	A927	U931	U932	A933	U934	A941	C946	A947	C948	U946	U947	U948	U949	U950	C951	U952	G956	G957	G958	G959	C965	A866	G969	U870	U871																							



• Molecule 23: 5S rRNA

Chain 5: 77% 21%



• Molecule 24: 50S ribosomal protein L1

Chain LA: 44% 9% 43%



- Molecule 25: 50S ribosomal protein L2

Chain LB: 93% 6% .



- Molecule 26: 50S ribosomal protein L3

Chain LC: 92% 8%



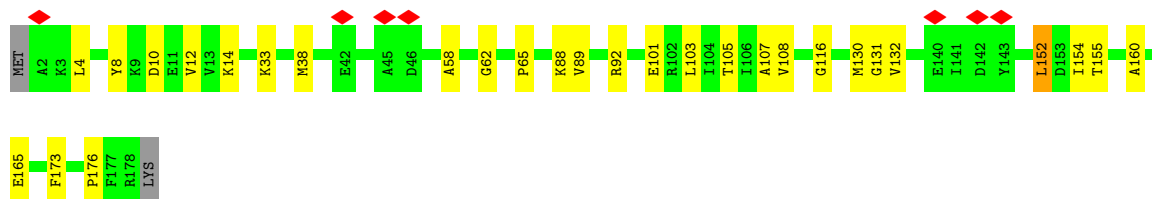
- Molecule 27: 50S ribosomal protein L4

Chain LD: 94% 6%



- Molecule 28: 50S ribosomal protein L5

Chain LE: 83% 16% ..

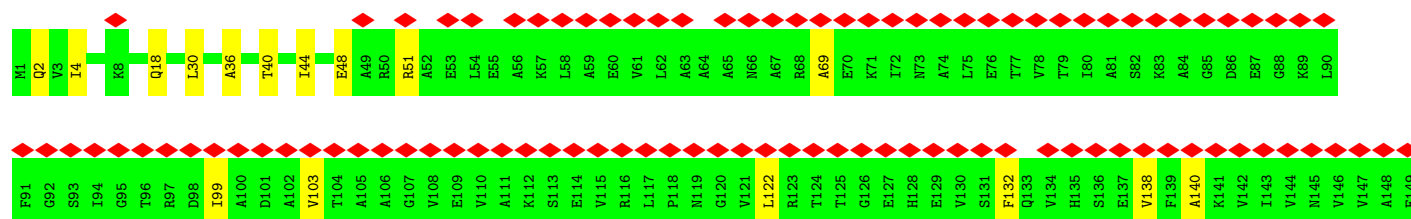
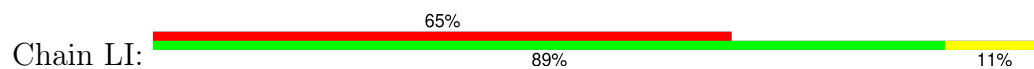


- Molecule 29: 50S ribosomal protein L6

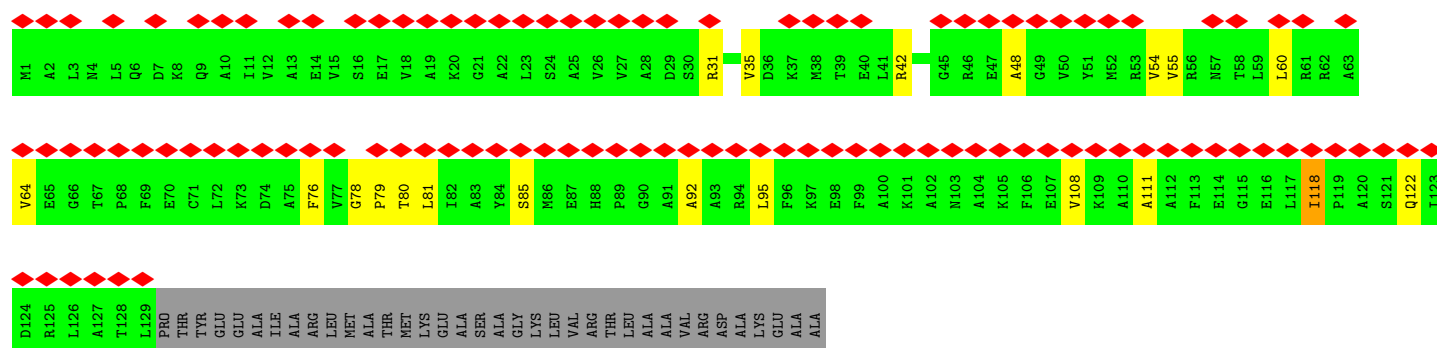
Chain LF: 86% 12% ..



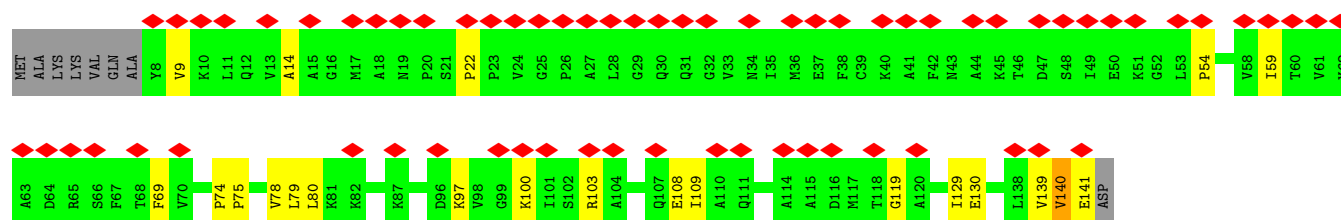
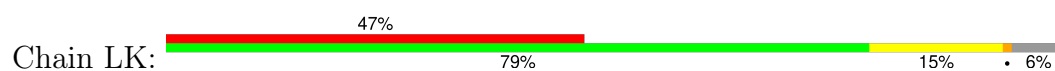
- Molecule 30: 50S ribosomal protein L9



- Molecule 31: 50S ribosomal protein L10



- Molecule 32: 50S ribosomal protein L11



- Molecule 33: 50S ribosomal protein L13



- Molecule 34: 50S ribosomal protein L14

Chain LN:  88% 11%



- Molecule 35: 50S ribosomal protein L15

Chain LO:  88% 11%



- Molecule 36: 50S ribosomal protein L16

Chain LP:  93% 7%



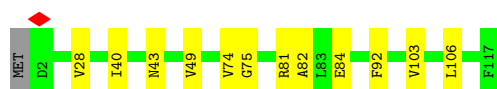
- Molecule 37: 50S ribosomal protein L17

Chain LQ:  88% 6% 6%



- Molecule 38: 50S ribosomal protein L18

Chain LR:  89% 10%



- Molecule 39: 50S ribosomal protein L19

Chain LS:  93% 6%



- Molecule 40: 50S ribosomal protein L20

Chain LT:  92% 7%



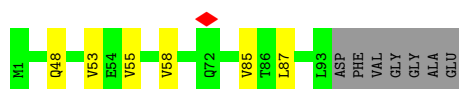
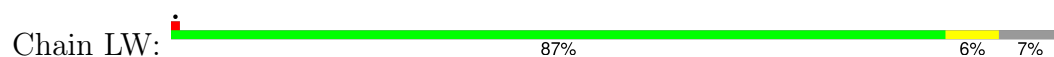
- Molecule 41: Ribosomal protein L21



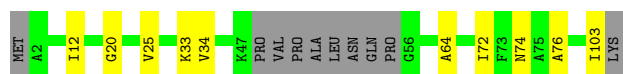
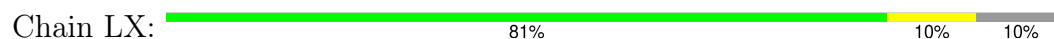
- Molecule 42: 50S ribosomal protein L22



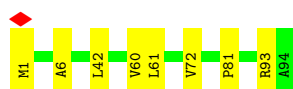
- Molecule 43: 50S ribosomal protein L23



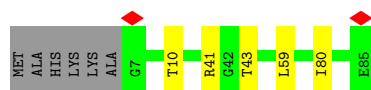
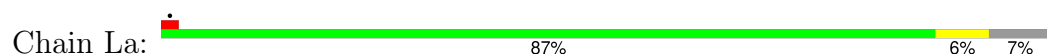
- Molecule 44: 50S ribosomal protein L24



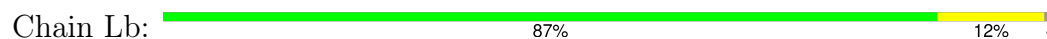
- Molecule 45: 50S ribosomal protein L25



- Molecule 46: 50S ribosomal protein L27

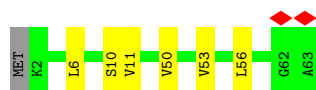


- Molecule 47: 50S ribosomal protein L28



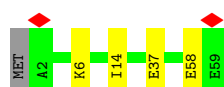
- Molecule 48: 50S ribosomal protein L29

Chain Lc:  89% 10%



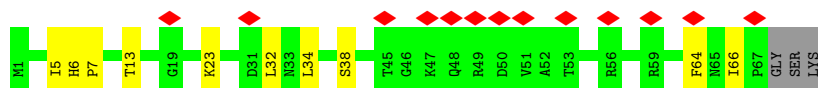
- Molecule 49: 50S ribosomal protein L30

Chain Ld:  92% 7%



- Molecule 50: 50S ribosomal protein L31

Chain Le:  19% 81% 14%



- Molecule 51: 50S ribosomal protein L32

Chain Lf:  81% 16%

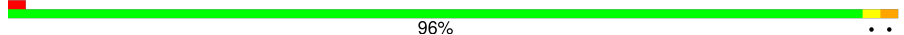


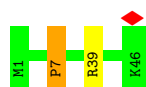
- Molecule 52: 50S ribosomal protein L33

Chain Lg:  85% 5% 9%



- Molecule 53: 50S ribosomal protein L34

Chain Lh:  96%



- Molecule 54: 50S ribosomal protein L35

Chain Li:  88% 9%



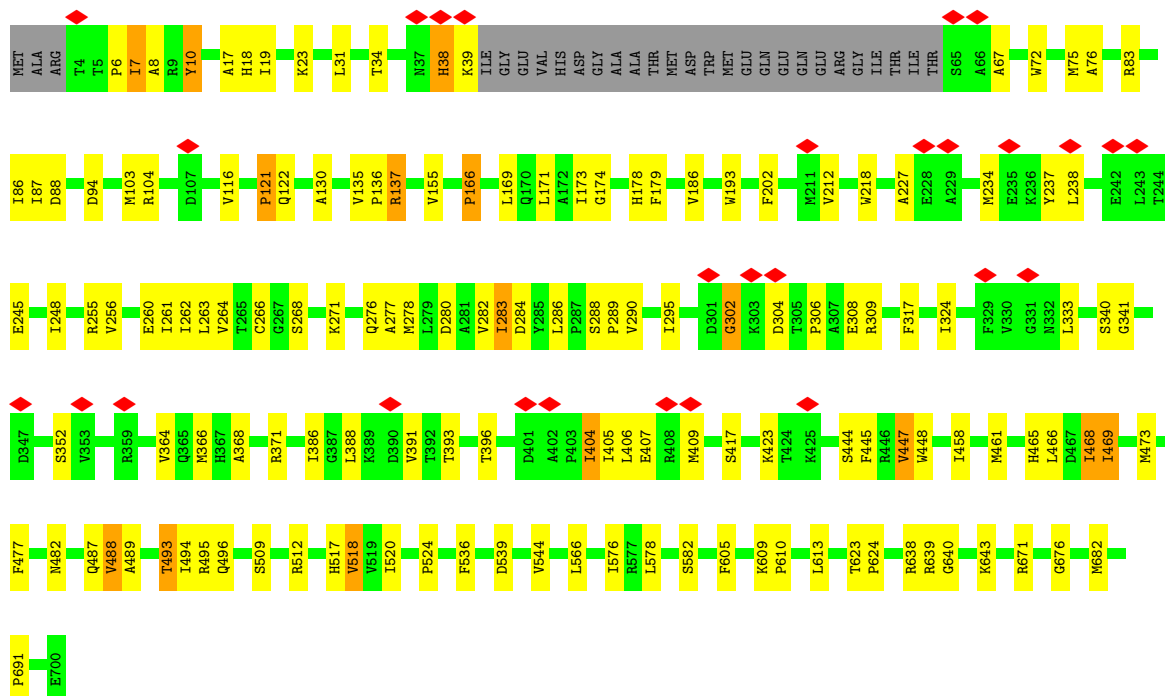
- Molecule 55: 50S ribosomal protein L36

Chain Lj: 95% 5%



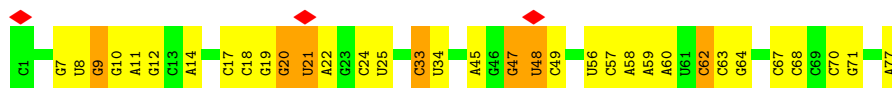
- Molecule 56: Elongation factor G

Chain EF: 75% 19%



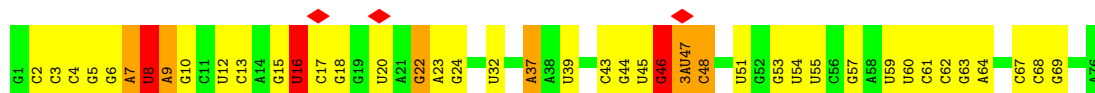
- Molecule 57: tRNA-fMet

Chain Dt: 56% 35% 9%

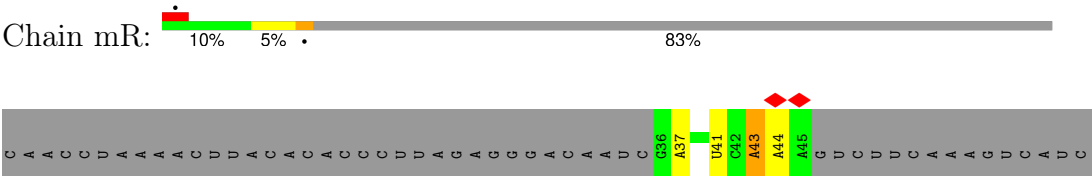


- Molecule 58: tRNA-Phe

Chain Pt: 45% 43% 8%



● Molecule 59: mRNA



● Molecule 60: Argyrin B



4 Experimental information

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 ($e^-/\text{\AA}^2$)	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 ⓘ

5.1 Standard geometry ⓘ

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

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(°)	Ideal(°)
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

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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 ⓘ

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 ⓘ

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 ⓘ

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$
22	PSU	23	746	62,22	18,21,22	1.43	3 (16%)	21,30,33	1.97	3 (14%)
22	6MZ	23	2030	22	22,25,26	1.48	5 (22%)	29,36,39	2.56	11 (37%)
1	5MC	16	1407	1	19,22,23	1.53	3 (15%)	26,32,35	1.26	3 (11%)
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	G7M	23	2069	22	23,26,27	2.38	5 (21%)	34,39,42	3.11	12 (35%)
60	BB9	B	2	60	2,5,6	3.25	1 (50%)	1,5,7	4.02	1 (100%)
22	OMG	23	2251	62,22,58	23,26,27	1.24	3 (13%)	32,38,41	2.10	7 (21%)
22	OMC	23	2498	62,22	19,22,23	0.85	0	25,31,34	0.82	0
1	MA6	16	1519	1	23,26,27	1.50	5 (21%)	33,38,41	2.13	11 (33%)
1	2MG	16	1516	1	23,26,27	1.25	4 (17%)	33,38,41	2.33	9 (27%)
22	OMU	23	2552	62,22	19,22,23	1.29	3 (15%)	25,31,34	1.99	5 (20%)
22	1MG	23	745	22	23,26,27	1.19	3 (13%)	33,39,42	1.72	6 (18%)
58	3AU	Pt	47	58	24,28,29	1.05	1 (4%)	30,40,43	1.41	4 (13%)
22	2MG	23	1835	22	23,26,27	1.26	3 (13%)	33,38,41	2.36	10 (30%)
58	G7M	Pt	46	58	23,26,27	2.38	5 (21%)	34,39,42	3.20	12 (35%)
1	G7M	16	527	1	23,26,27	2.37	5 (21%)	34,39,42	3.05	11 (32%)
58	PSU	Pt	39	58	18,21,22	1.36	2 (11%)	21,30,33	2.07	4 (19%)
22	5MU	23	747	22	19,22,23	1.48	6 (31%)	27,32,35	2.15	7 (25%)
22	2MA	23	2503	62,22	22,25,26	1.53	4 (18%)	32,37,40	2.44	8 (25%)
36	4D4	LP	81	36	9,11,12	3.18	3 (33%)	7,13,15	3.43	3 (42%)
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	4SU	Pt	8	58	18,21,22	1.91	5 (27%)	25,30,33	2.34	5 (20%)
57	4SU	Dt	8	57	18,21,22	1.88	5 (27%)	25,30,33	2.22	5 (20%)
57	PSU	Dt	56	57	18,21,22	1.43	2 (11%)	21,30,33	2.10	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
60	DHA	B	7	60	3,4,5	4.88	1 (33%)	2,4,6	4.07	2 (100%)
1	PSU	16	516	1	18,21,22	1.42	3 (16%)	21,30,33	2.31	5 (23%)
22	5MC	23	1962	62,22	19,22,23	1.55	3 (15%)	26,32,35	1.30	2 (7%)
22	5MU	23	1939	62,22	19,22,23	1.44	5 (26%)	27,32,35	2.21	6 (22%)
1	UR3	16	1498	1	19,22,23	0.96	0	26,32,35	1.84	3 (11%)
22	2MG	23	2445	62,22	23,26,27	1.27	4 (17%)	33,38,41	2.29	10 (30%)
22	PSU	23	1917	22	18,21,22	1.48	3 (16%)	21,30,33	2.09	4 (19%)
1	5MC	16	967	1	19,22,23	1.62	3 (15%)	26,32,35	1.75	7 (26%)
22	PSU	23	2580	22	18,21,22	1.52	4 (22%)	21,30,33	2.17	5 (23%)
1	2MG	16	966	1	23,26,27	1.27	3 (13%)	33,38,41	2.25	10 (30%)
57	OMC	Dt	33	57	19,22,23	0.85	0	25,31,34	0.88	1 (4%)
58	H2U	Pt	16	58	18,21,22	1.14	3 (16%)	19,30,33	1.18	1 (5%)
60	SAR	B	8	60	3,4,5	1.04	0	1,3,5	1.88	0
22	H2U	23	2449	22	18,21,22	1.16	3 (16%)	19,30,33	1.11	1 (5%)
22	PSU	23	1911	22	18,21,22	1.41	3 (16%)	21,30,33	2.05	3 (14%)
58	MIA	Pt	37	58	28,31,32	2.30	7 (25%)	38,44,47	2.85	15 (39%)
1	4OC	16	1402	1	20,23,24	0.79	0	25,32,35	1.09	1 (4%)
22	3TD	23	1915	22	19,22,23	1.26	2 (10%)	23,32,35	2.04	3 (13%)
58	PSU	Pt	55	58	18,21,22	1.39	2 (11%)	21,30,33	2.07	3 (14%)
57	H2U	Dt	21	57	18,21,22	1.06	3 (16%)	19,30,33	1.52	5 (26%)
1	MA6	16	1518	1	23,26,27	1.52	5 (21%)	33,38,41	2.15	11 (33%)
22	PSU	23	2604	22	18,21,22	1.52	3 (16%)	21,30,33	2.20	5 (23%)
22	PSU	23	955	22	18,21,22	1.48	4 (22%)	21,30,33	2.20	3 (14%)
22	6MZ	23	1618	22	22,25,26	1.47	5 (22%)	29,36,39	2.20	10 (34%)
12	D2T	SL	89	12	8,9,10	3.34	2 (25%)	6,11,13	2.06	2 (33%)
22	PSU	23	2457	22	18,21,22	1.57	4 (22%)	21,30,33	2.20	6 (28%)
60	0UO	B	4	60	16,17,18	1.53	5 (31%)	17,23,25	1.73	5 (29%)
22	PSU	23	2504	22	18,21,22	1.48	4 (22%)	21,30,33	2.21	5 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	PSU	23	746	62,22	-	1/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	6MZ	23	2030	22	-	1/9/27/28	0/3/3/3
1	5MC	16	1407	1	-	0/7/25/26	0/2/2/2
60	DBB	B	6	60	-	1/3/4/6	-
57	G7M	Dt	47	57	-	0/7/25/26	0/3/3/3
22	G7M	23	2069	22	-	2/7/25/26	0/3/3/3
60	BB9	B	2	60	-	0/0/4/6	-
22	OMG	23	2251	62,22,58	-	3/9/27/28	0/3/3/3
22	OMC	23	2498	62,22	-	2/9/27/28	0/2/2/2
1	MA6	16	1519	1	-	0/11/29/30	0/3/3/3
1	2MG	16	1516	1	-	0/9/27/28	0/3/3/3
22	OMU	23	2552	62,22	-	0/9/27/28	0/2/2/2
22	1MG	23	745	22	-	0/7/25/26	0/3/3/3
58	3AU	Pt	47	58	-	6/16/34/35	0/2/2/2
22	2MG	23	1835	22	-	0/9/27/28	0/3/3/3
58	G7M	Pt	46	58	-	0/7/25/26	0/3/3/3
1	G7M	16	527	1	-	2/7/25/26	0/3/3/3
58	PSU	Pt	39	58	-	0/7/25/26	0/2/2/2
22	5MU	23	747	22	-	2/7/25/26	0/2/2/2
22	2MA	23	2503	62,22	-	2/7/25/26	0/3/3/3
36	4D4	LP	81	36	-	3/11/12/14	-
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	4SU	Pt	8	58	-	3/7/25/26	0/2/2/2
57	4SU	Dt	8	57	-	0/7/25/26	0/2/2/2
57	PSU	Dt	56	57	-	0/7/25/26	0/2/2/2
60	DHA	B	7	60	-	0/0/2/4	-
1	PSU	16	516	1	-	0/7/25/26	0/2/2/2
22	5MC	23	1962	62,22	-	0/7/25/26	0/2/2/2
22	5MU	23	1939	62,22	-	0/7/25/26	0/2/2/2
1	UR3	16	1498	1	-	0/7/25/26	0/2/2/2
22	2MG	23	2445	62,22	-	1/9/27/28	0/3/3/3
22	PSU	23	1917	22	-	0/7/25/26	0/2/2/2
1	5MC	16	967	1	-	2/7/25/26	0/2/2/2
22	PSU	23	2580	22	-	0/7/25/26	0/2/2/2
1	2MG	16	966	1	-	1/9/27/28	0/3/3/3
57	OMC	Dt	33	57	-	1/9/27/28	0/2/2/2
58	H2U	Pt	16	58	-	0/7/38/39	0/2/2/2
60	SAR	B	8	60	-	1/1/2/3	-
22	H2U	23	2449	22	-	0/7/38/39	0/2/2/2
22	PSU	23	1911	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
58	MIA	Pt	37	58	-	3/15/33/34	0/3/3/3
1	4OC	16	1402	1	-	1/9/29/30	0/2/2/2
22	3TD	23	1915	22	-	0/7/25/26	0/2/2/2
58	PSU	Pt	55	58	-	0/7/25/26	0/2/2/2
57	H2U	Dt	21	57	-	1/7/38/39	0/2/2/2
1	MA6	16	1518	1	-	0/11/29/30	0/3/3/3
22	PSU	23	2604	22	-	0/7/25/26	0/2/2/2
22	PSU	23	955	22	-	0/7/25/26	0/2/2/2
22	6MZ	23	1618	22	-	0/9/27/28	0/3/3/3
12	D2T	SL	89	12	-	2/7/12/14	-
22	PSU	23	2457	22	-	0/7/25/26	0/2/2/2
60	0UO	B	4	60	-	2/7/8/10	0/2/2/2
22	PSU	23	2504	22	-	0/7/25/26	0/2/2/2

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	Pt	46	G7M	C5-N7	-4.26	1.34	1.39
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23	1835	2MG	C5-C4	2.90	1.46	1.38
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16	967	5MC	C6-N1	-2.48	1.33	1.38
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	16	516	PSU	C2-N3	-2.15	1.33	1.37
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(°)	Ideal(°)
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23	2503	2MA	N3-C4-N9	6.93	135.78	126.99
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	Pt	46	G7M	C5-C4-N3	-5.13	118.47	128.15
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23	2457	PSU	C4-N3-C2	-4.18	120.61	126.37
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23	2580	PSU	O2-C2-N1	-3.65	119.02	122.79
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	B	4	0UO	O3-C17-C16	-3.02	119.21	124.30
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	Dt	47	G7M	O4'-C1'-N9	2.45	113.91	108.36
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23	1618	6MZ	O3'-C3'-C2'	-2.18	104.81	111.82
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'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
58	Pt	47	3AU	O4'-C4'-C5'-O5'
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
22	23	2030	6MZ	1	0
60	B	6	DBB	2	0
57	Dt	47	G7M	1	0
60	B	2	BB9	1	0
22	23	2251	OMG	1	0
58	Pt	46	G7M	1	0
58	Pt	8	4SU	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	B	7	DHA	3	0
1	16	516	PSU	1	0
57	Dt	33	OMC	1	0
58	Pt	16	H2U	1	0
60	B	8	SAR	4	0
58	Pt	37	MIA	1	0
1	16	1518	MA6	2	0
60	B	4	0UO	2	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	3007	-	5,5,5	0.15	0	4,4,4	0.22	0
65	GDP	EF	801	-	29,30,30	1.15	4 (13%)	45,47,47	1.76	5 (11%)
66	FME	Pt	3001	67	8,9,10	0.55	0	8,9,11	1.52	2 (25%)
61	PUT	23	3005	-	5,5,5	0.15	0	4,4,4	0.23	0
61	PUT	23	3006	-	5,5,5	0.15	0	4,4,4	0.20	0
61	PUT	23	3001	-	5,5,5	0.15	0	4,4,4	0.26	0
61	PUT	23	3009	-	5,5,5	0.15	0	4,4,4	0.21	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
61	PUT	16	1601	-	5,5,5	0.14	0	4,4,4	0.21	0
61	PUT	23	3008	-	5,5,5	0.15	0	4,4,4	0.20	0
61	PUT	23	3003	-	5,5,5	0.14	0	4,4,4	0.23	0
63	SPD	23	3011	-	9,9,9	0.15	0	8,8,8	0.25	0
67	PHE	Pt	3002	58,66	8,9,12	3.35	3 (37%)	3,10,15	4.30	3 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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

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	3007	-	-	0/3/3/3	-
65	GDP	EF	801	-	-	0/16/32/32	0/3/3/3
66	FME	Pt	3001	67	-	5/7/9/11	-
61	PUT	23	3005	-	-	1/3/3/3	-
61	PUT	23	3006	-	-	0/3/3/3	-
61	PUT	23	3001	-	-	0/3/3/3	-
61	PUT	23	3009	-	-	0/3/3/3	-
63	SPD	23	3010	-	-	1/7/7/7	-
61	PUT	23	3002	-	-	1/3/3/3	-
61	PUT	16	1601	-	-	0/3/3/3	-
61	PUT	23	3008	-	-	0/3/3/3	-
61	PUT	23	3003	-	-	0/3/3/3	-
63	SPD	23	3011	-	-	0/7/7/7	-
67	PHE	Pt	3002	58,66	-	4/8/6/8	-
61	PUT	16	1602	-	-	0/3/3/3	-
61	PUT	23	3004	-	-	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(°)	Ideal(°)
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
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

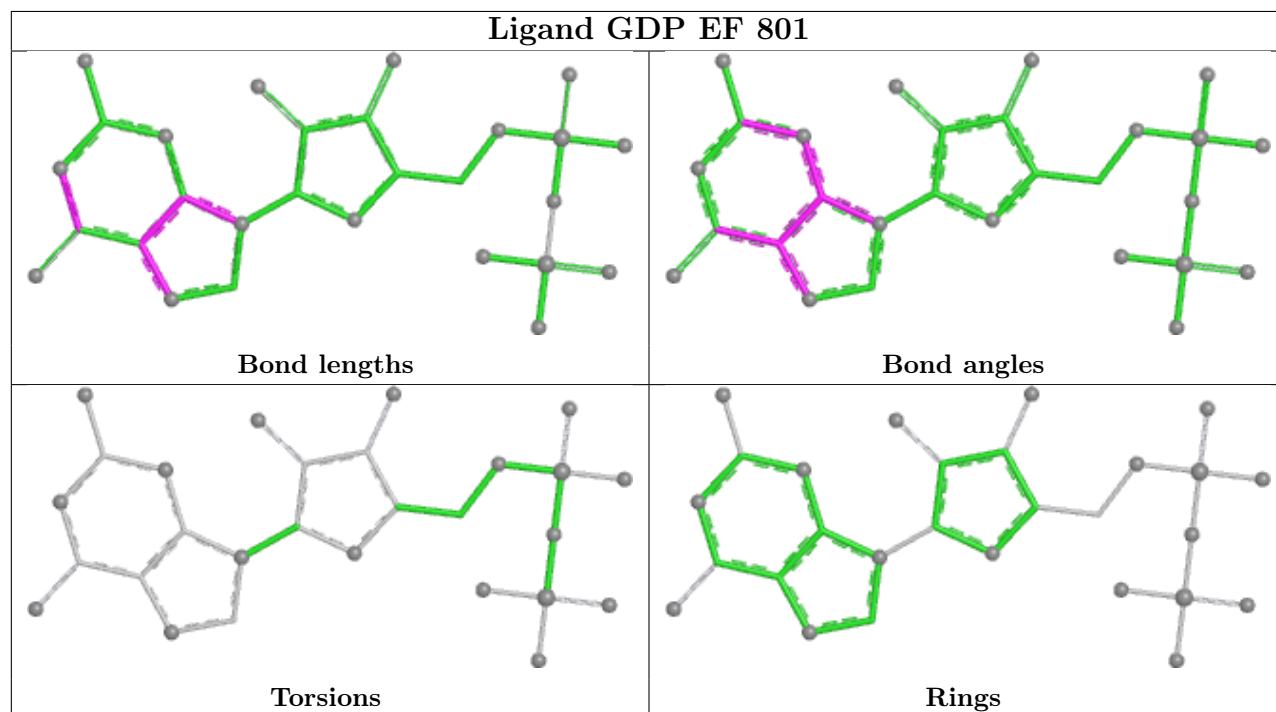
There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	16	1601	PUT	1	0
63	23	3011	SPD	1	0
67	Pt	3002	PHE	1	0
61	23	3004	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

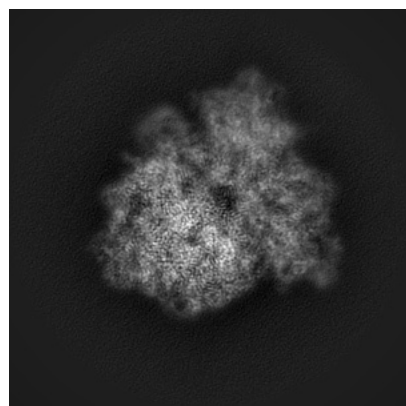
6 Map visualisation [i](#)

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.

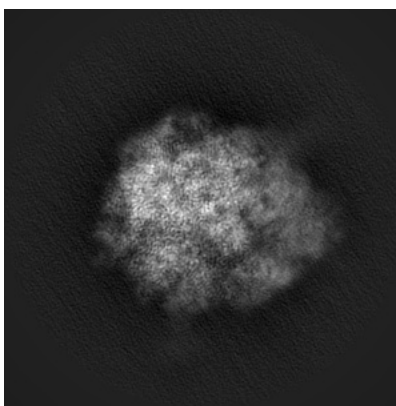
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

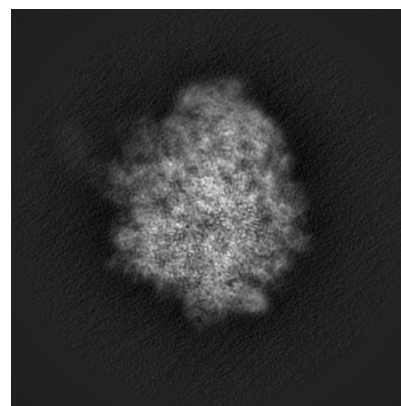
6.1.1 Primary map



X

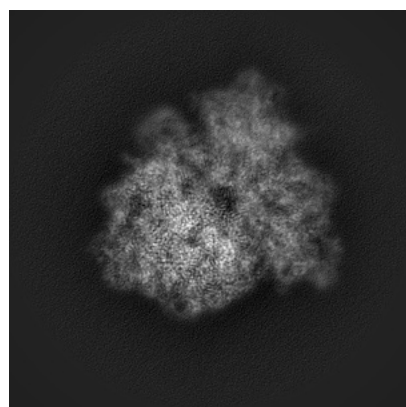


Y

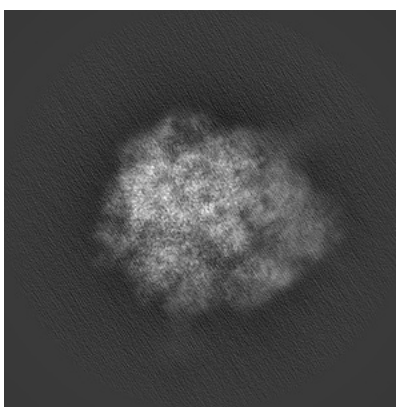


Z

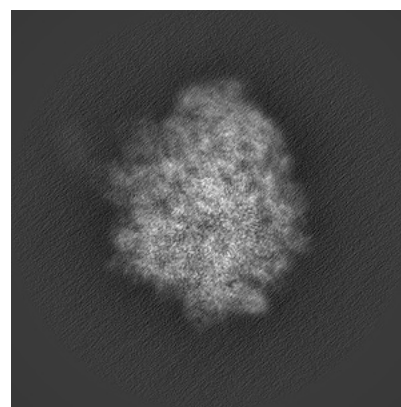
6.1.2 Raw map



X



Y

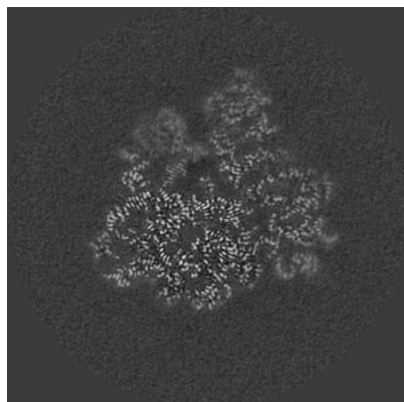


Z

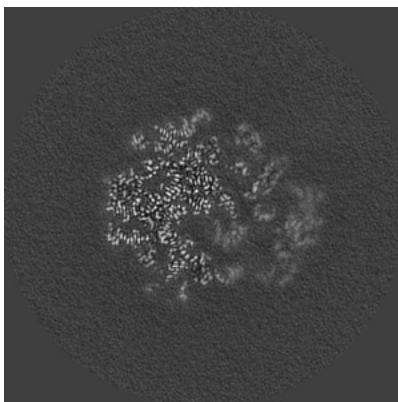
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

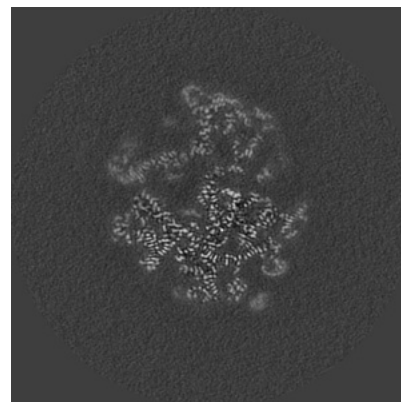
6.2.1 Primary map



X Index: 190

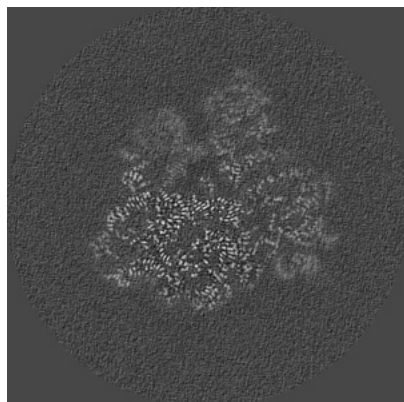


Y Index: 190

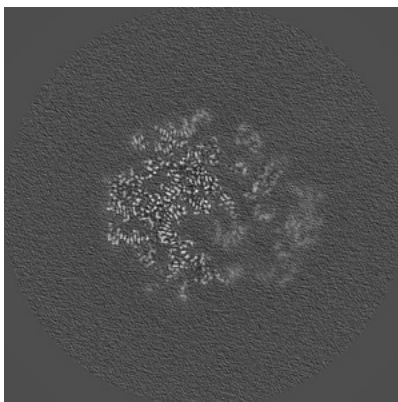


Z Index: 190

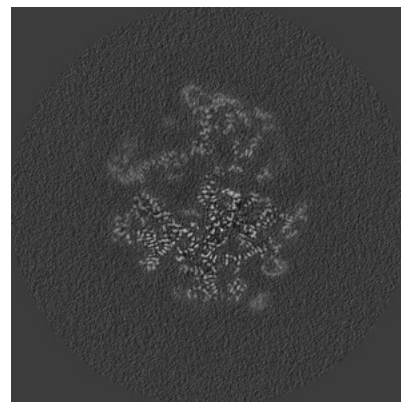
6.2.2 Raw map



X Index: 190



Y Index: 190

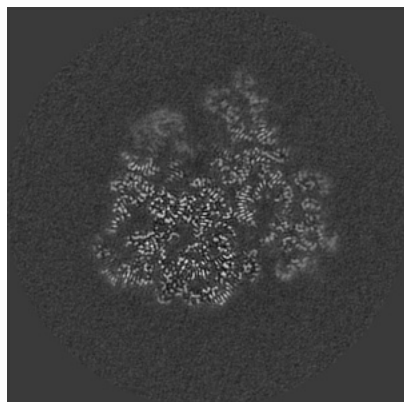


Z Index: 190

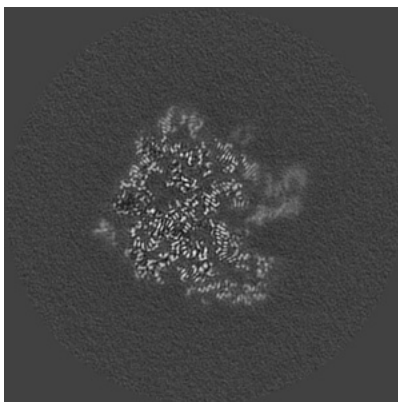
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

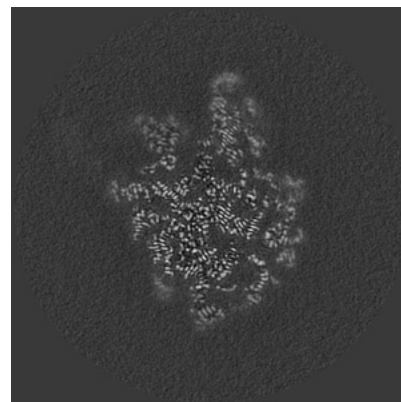
6.3.1 Primary map



X Index: 195

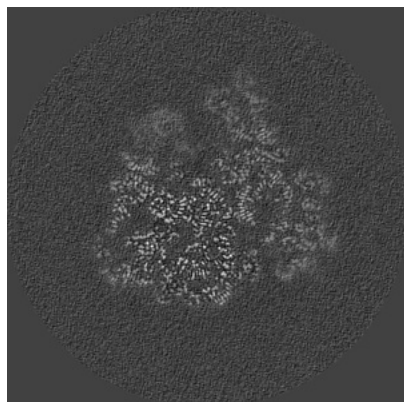


Y Index: 157

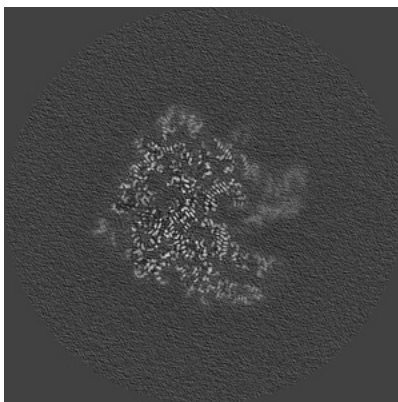


Z Index: 153

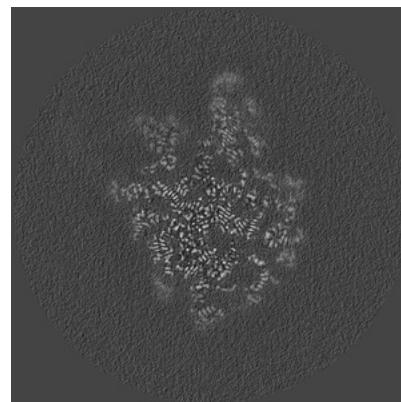
6.3.2 Raw map



X Index: 195



Y Index: 158

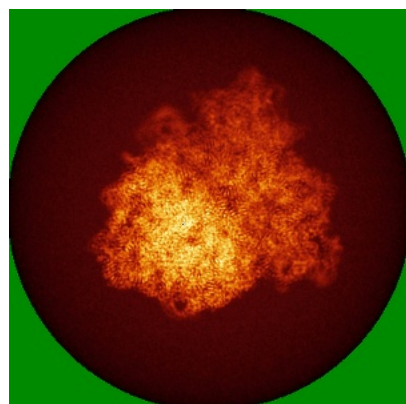


Z Index: 153

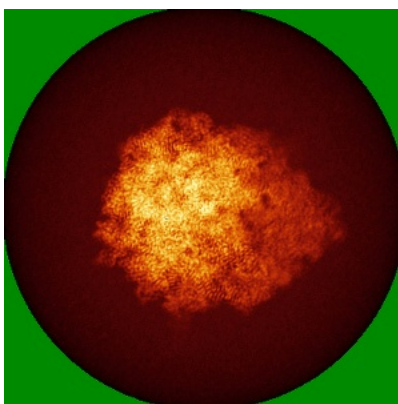
The images above show the largest variance slices of the map in three orthogonal directions.

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

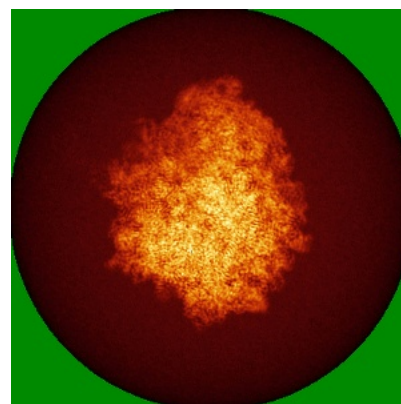
6.4.1 Primary map



X

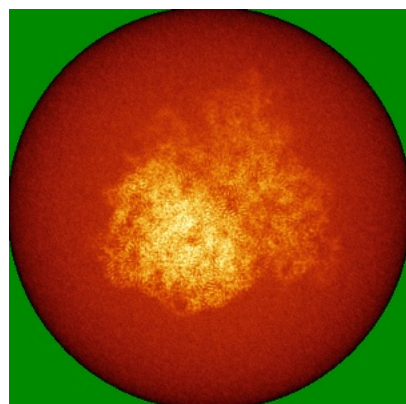


Y

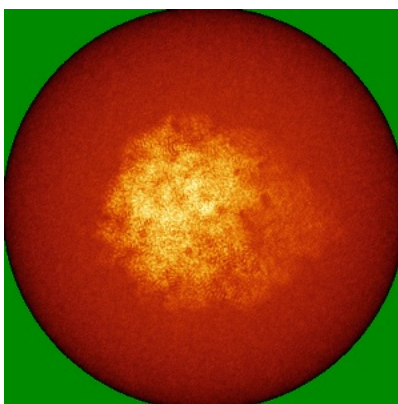


Z

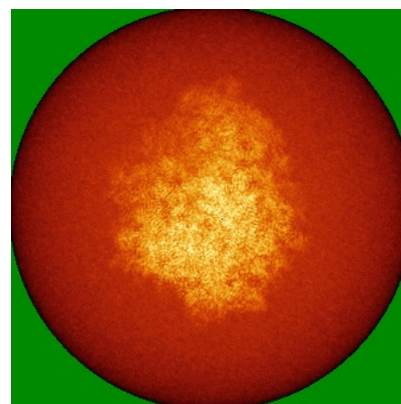
6.4.2 Raw map



X



Y

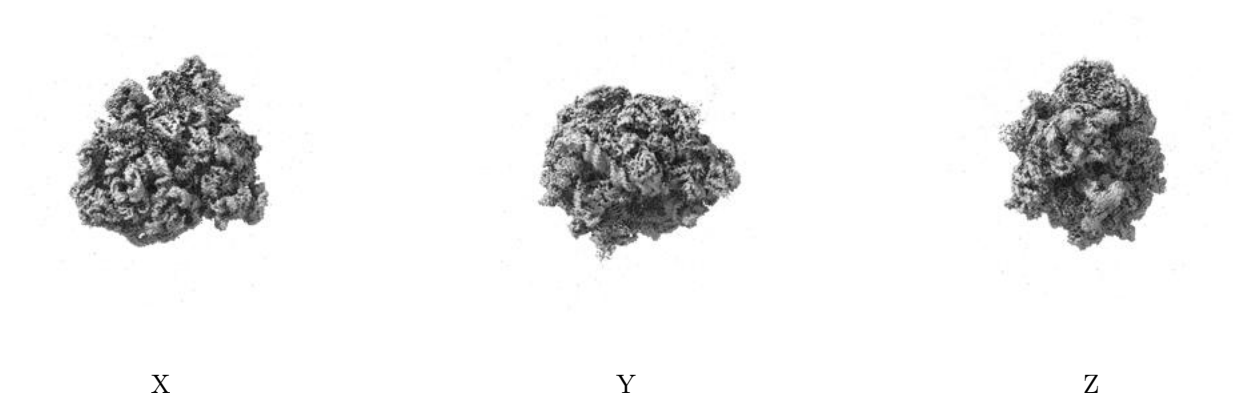


Z

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.

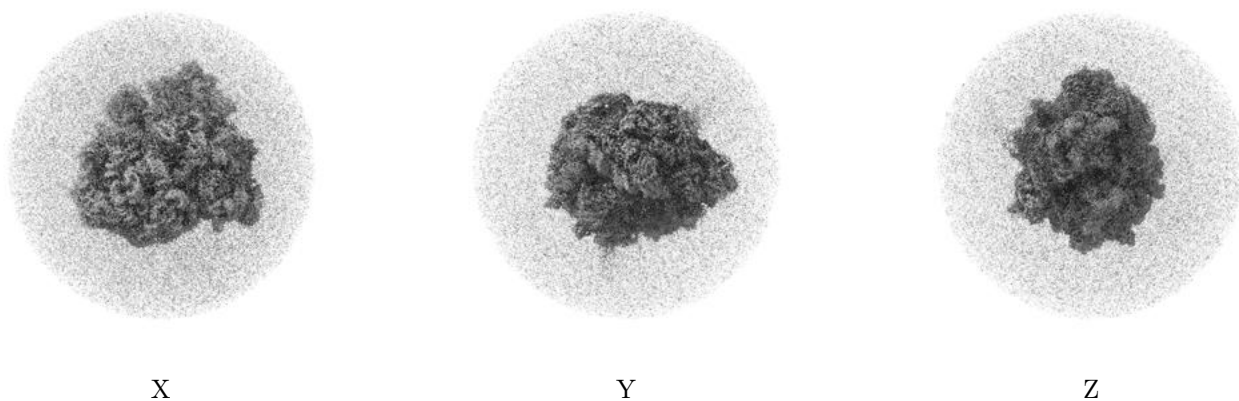
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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



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.

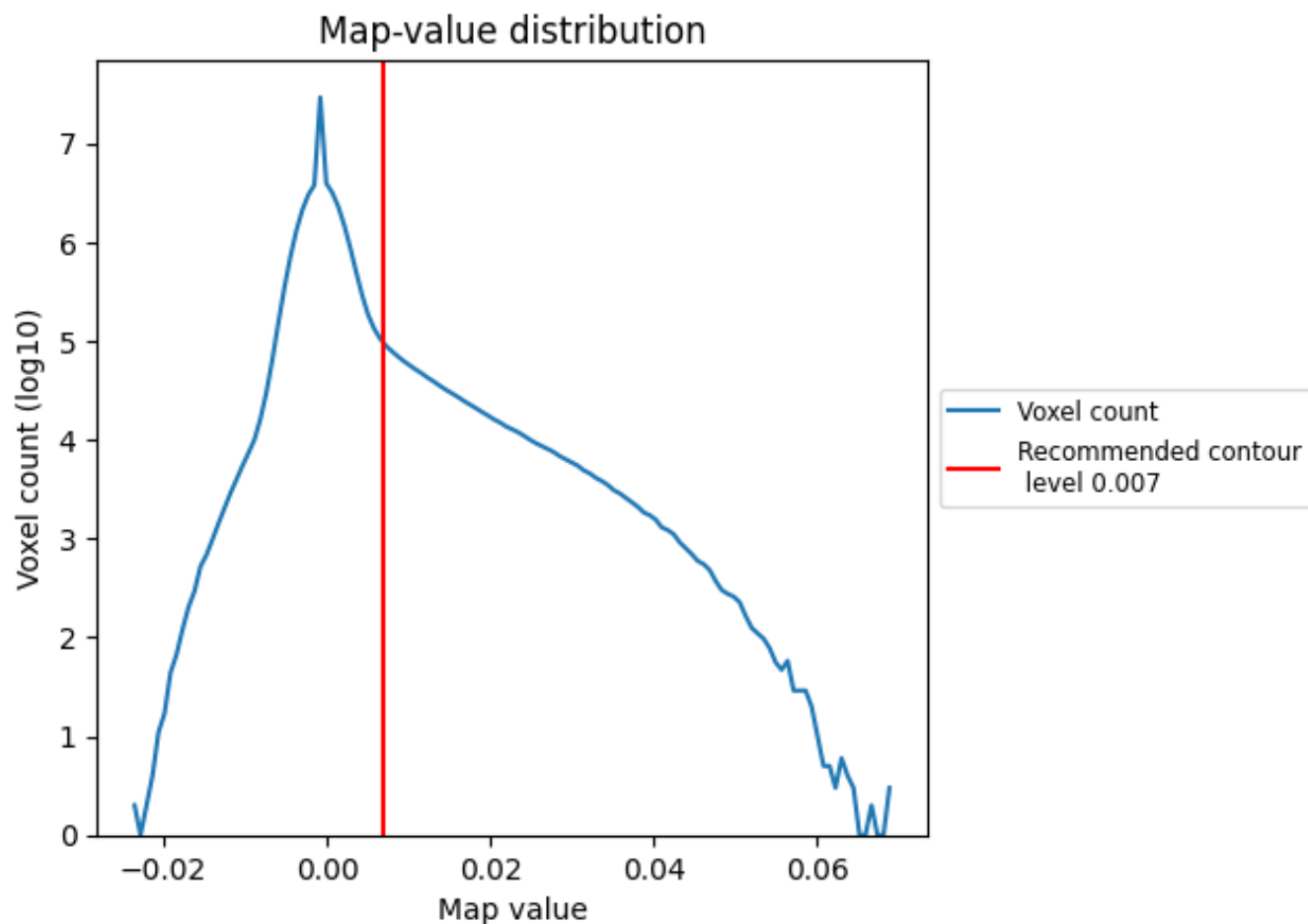
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

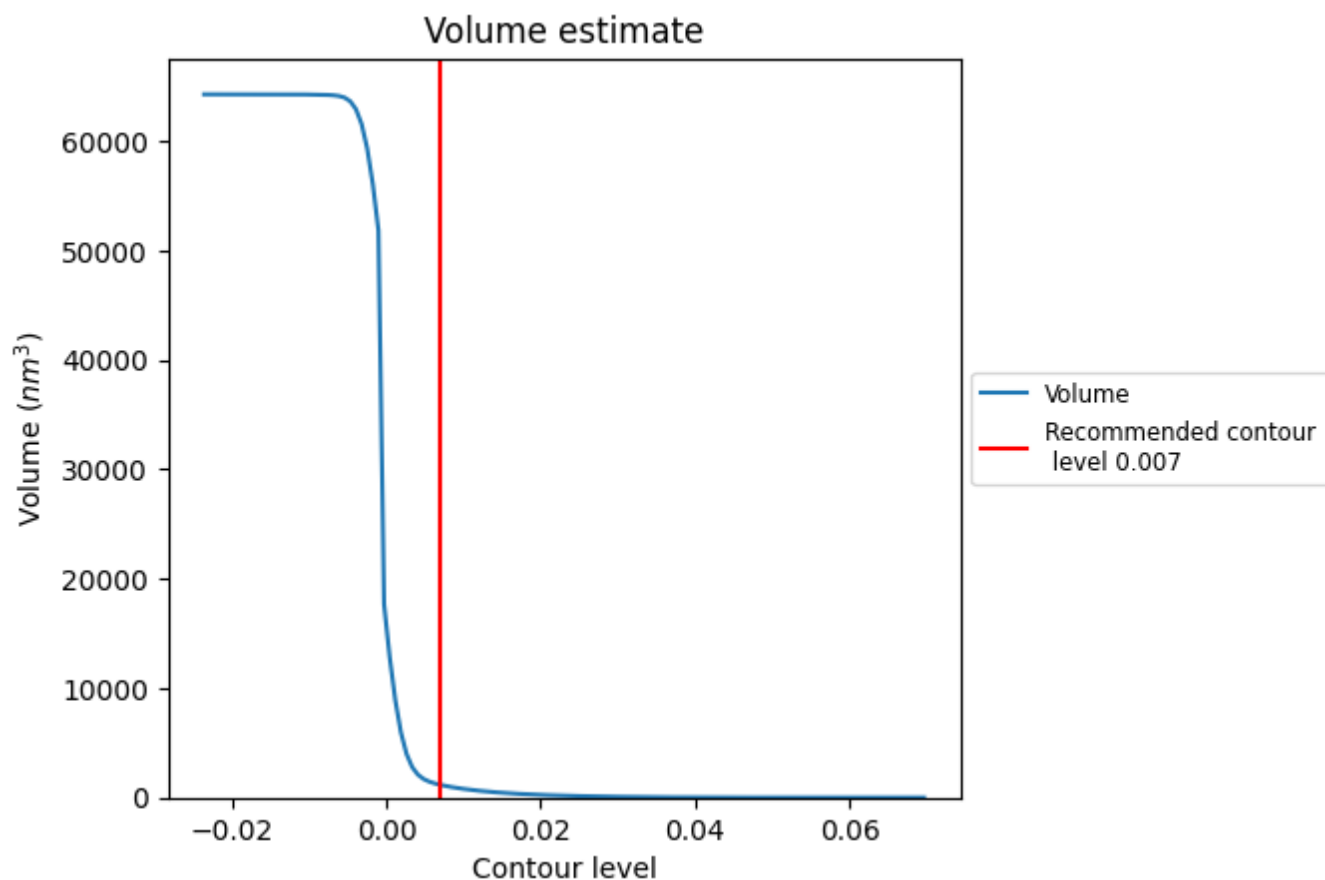
This section contains the results of statistical analysis of the map.

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.

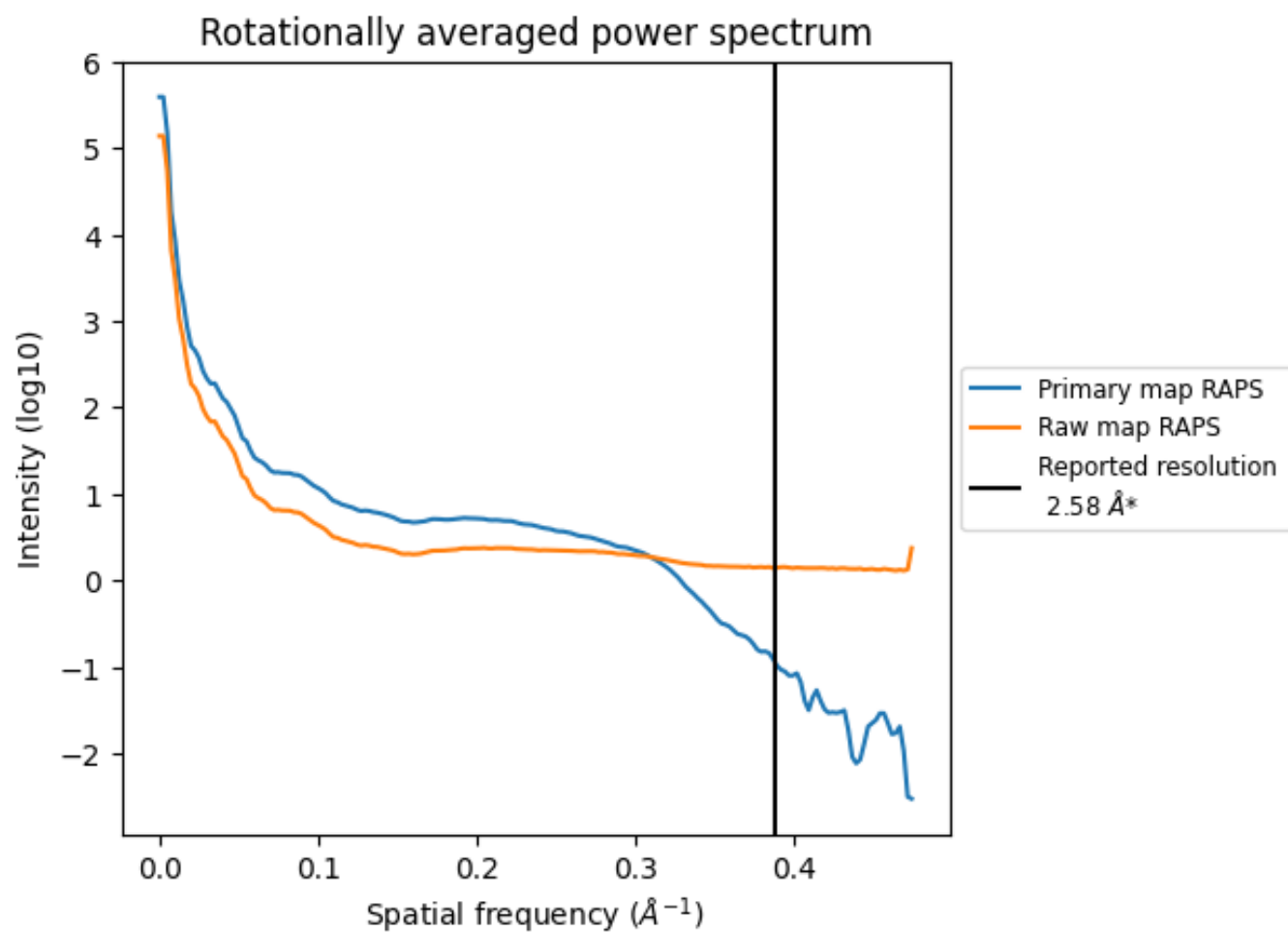
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1165 nm³; 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 ⓘ

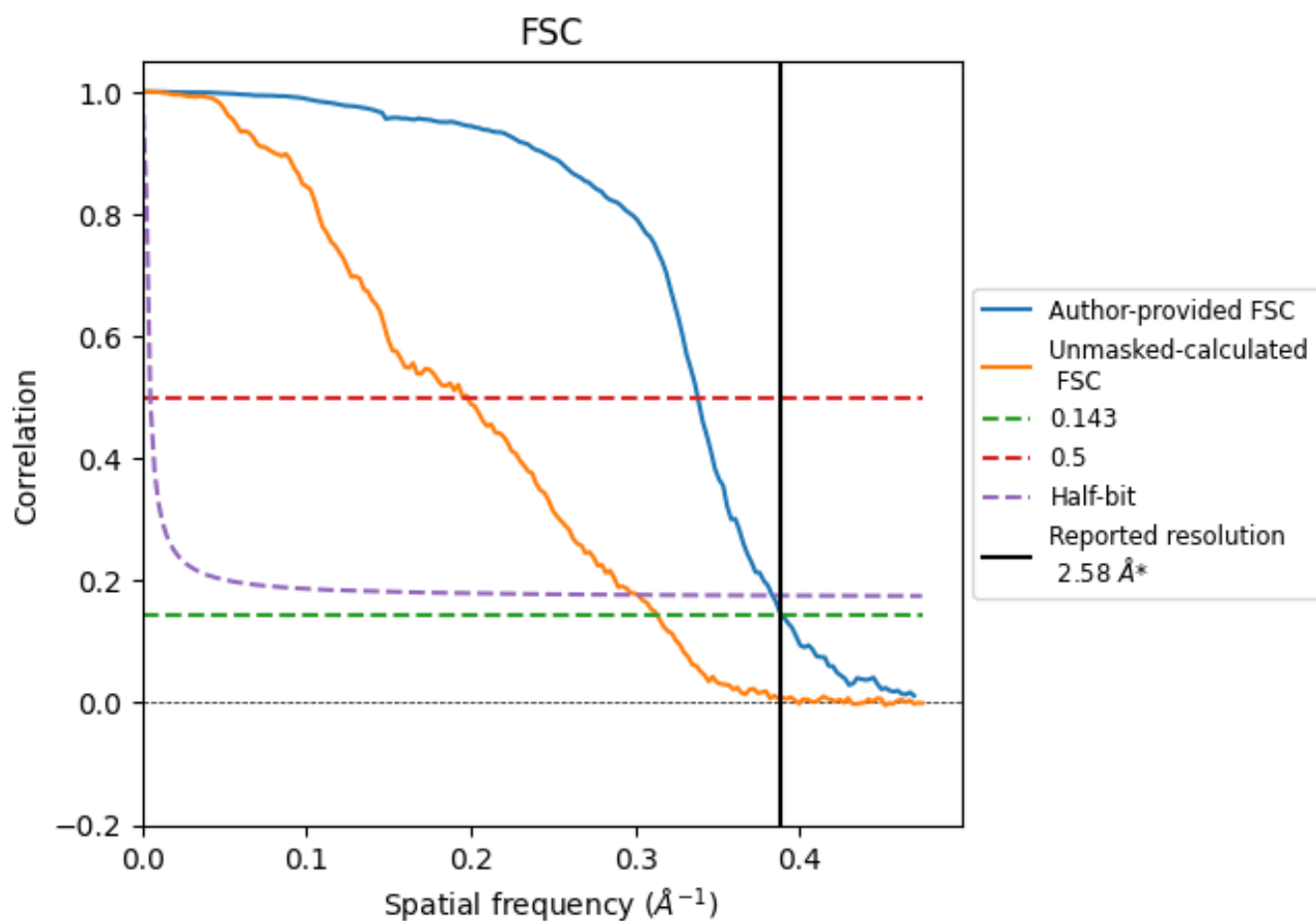


*Reported resolution corresponds to spatial frequency of 0.388 Å⁻¹

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 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

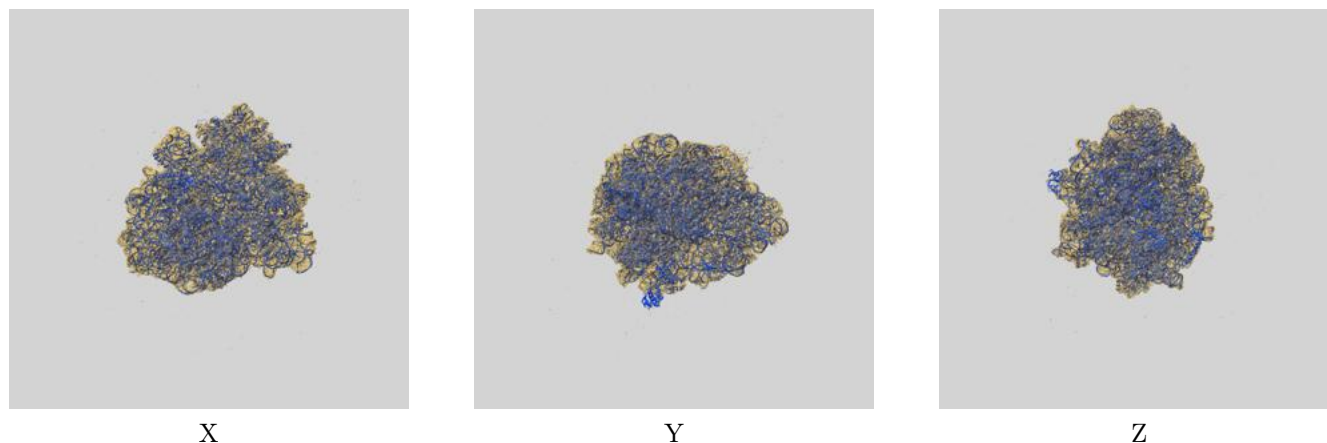
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.58	-	-
Author-provided FSC curve	2.57	2.96	2.61
Unmasked-calculated*	3.19	5.06	3.32

*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](#)

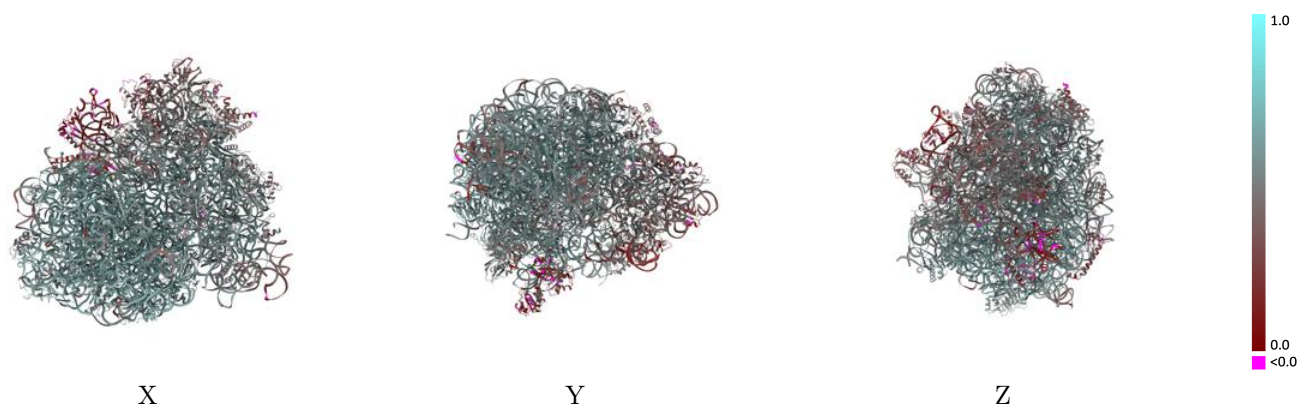
This section contains information regarding the fit between EMDB map EMD-26486 and PDB model 7UG7. Per-residue inclusion information can be found in section 3 on page 19.

9.1 Map-model overlay [i](#)



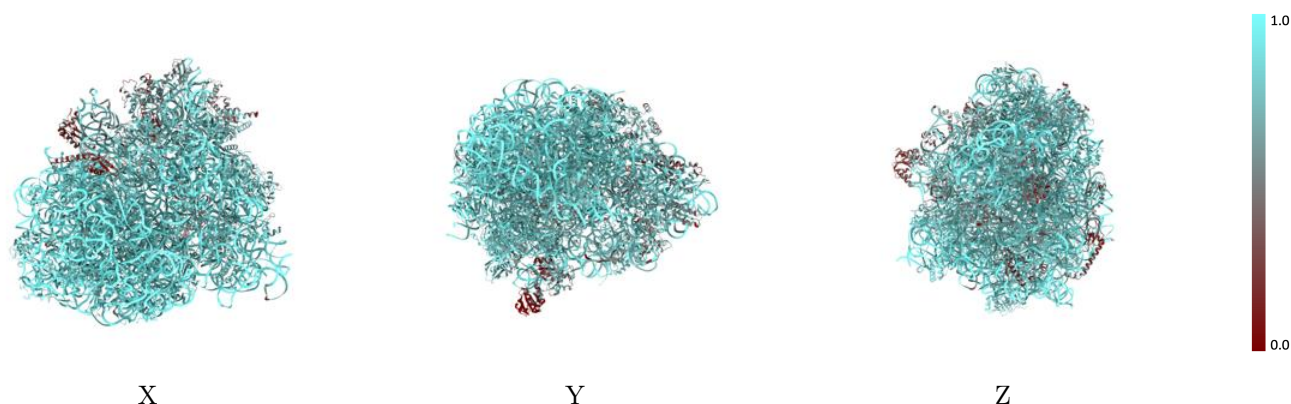
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



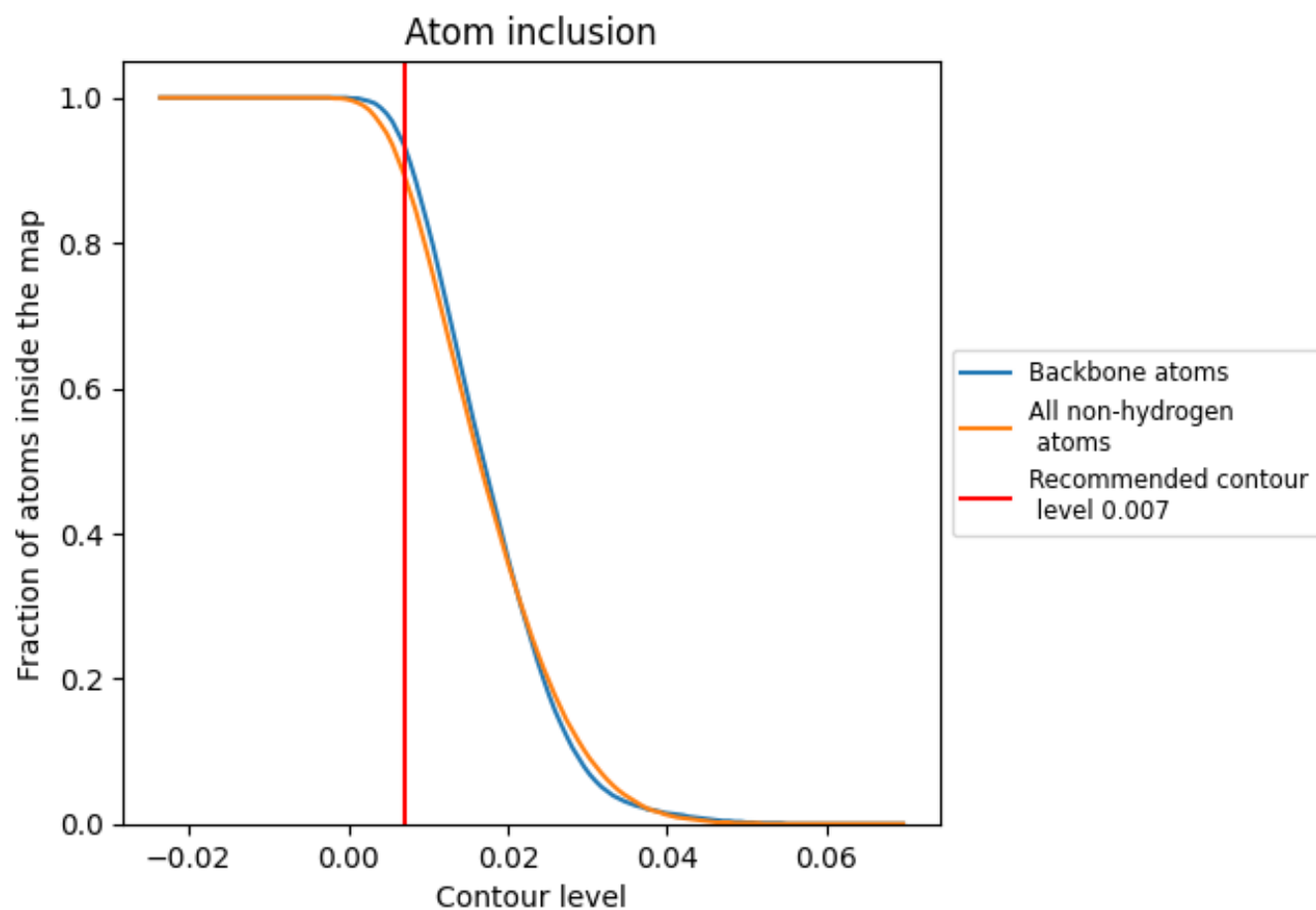
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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