

# Full wwPDB X-ray Structure Validation Report (i)

#### Sep 14, 2023 – 01:59 AM EDT

PDB ID	:	4V4J
Title	:	Interactions and Dynamics of the Shine-Dalgarno Helix in the 70S Ribosome.
Authors	:	Korostelev, A.; Trakhanov, S.; Asahara, H.; Laurberg, M.; Noller, H.F.
Deposited on	:	2007-07-18
Resolution	:	3.83  Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY\;DIFFRACTION$ 

The reported resolution of this entry is 3.83 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R <sub>free</sub>	130704	$1242 \ (4.08-3.60)$
Ramachandran outliers	138981	$1003 \ (4.06-3.62)$
Sidechain outliers	138945	1266 (4.08-3.60)
RSRZ outliers	127900	1149 (4.08-3.60)
RNA backbone	3102	$1038 \ (4.68-3.00)$

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length		Qu	ality	of ch	ain		
1	W	2889	4%	65%				33%	•
2	х	120		61%			3	8%	•
3	А	229	3%		13%	•	45%	6	
4	В	276	7%	62%			34	1%	
5	С	206	6%	60%			33%		••



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Mol	Chain	Length	Quality of cha	in	
6	D	205	60%	32%	• 5%
7	F	189	4%		
		102	4%	23%	
8	F	180	67% 5%	29%	• •
9	G	148	66%	31%	•
10	Н	140	% 65%	31%	
11	Ι	122	56%	39%	•••
12	J	150	2% 64%	29%	
13	K	141	57%	36%	
14	T	118	5%	25%	
14		110	4%	23%	•
15	М	112	65% 2%	26%	• 5%
16	Ν	146	57%	34%	• 6%
17	О	118	69%	28%	••
18	Р	101	55%	40%	5%
19	Q	113	69%	24%	• •
20	R	96	% 61%	30%	• •
01	C	110	20%		
21	5	110	47%	43%	• 6%
22	Т	206	68%	19% •	• 10%
23	U	85	59%	27%	• 11%
24	V	98	63%	24%	• 10%
25	W	72	54%	26% 6%	14%
26	X	60	<u>80%</u>	1	.8% •
27	Y	60	65%	23%	5% 7%
28	Z	49	76%	20%	, ••
29	a	65	63%	34%	
20	L	07	30%		
- 30	a	31	73%	19%	• 5%



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Mol	Chain	Length	Quality of chai	n	
31	у	1522	4% 65%	32%	••
32	Z	77	5%	26%	%
33	2	76	9%	28%	
	_		33%		
34	3	18	72%	28%	
35	с	256	69%	20%	• 9%
36	d	239	59%	25% •	14%
37	е	209	3% 77%	21	% •
38	f	162	4%	14%	• 7%
39	g	101	2% <b>8</b> 1%	1	.7% •
	0		3%		
40	h	156	72%	25%	•••
41	i	138	72%	26%	•
42	j	128	81%	1	.7% ••
43	k	105	68%	25%	• 7%
44	1	129	9%	17%	10%
45	m	132	6%	33%	6%
			13%	5570	0,0
46	n	126	67%	29%	• •
47	0	61	3% 64%	30%	5% •
48	n	89	12%	22%	
40	P		24%	25%	604
49	q	00	56%	35%	• 6%
50	r	105	63%	33%	••
51	s	88	69%	22%	• 8%
52	t	93	46% 34	% 5%	14%
53	u	106	71%	22%	• 7%
54	v	27	48%	41%	11%



# 2 Entry composition (i)

There are 54 unique types of molecules in this entry. The entry contains 147125 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 23S LARGE SUBUNIT RIBOSOMAL RNA.

Mol	Chain	Residues			Atoms	ZeroOcc	AltConf	Trace		
1	W	2889	Total 62213	C 27690	N 11624	O 20011	Р 2888	0	0	0

• Molecule 2 is a RNA chain called 5S LARGE SUBUNIT RIBOSOMAL RNA.

Mol	Chain	Residues		At	toms		ZeroOcc	AltConf	Trace	
2	х	120	Total 2573	C 1146	N 476	O 832	Р 119	0	0	0

• Molecule 3 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	А	127	Total 996	C 627	N 184	0 184	S 1	0	0	0

• Molecule 4 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
4	В	272	Total 2115	C 1335	N 420	O 357	${ m S} { m 3}$	0	0	0

• Molecule 5 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	С	201	Total 1541	C 974	N 295	O 267	${ m S}{ m 5}$	0	0	0

• Molecule 6 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
6	D	194	Total 1517	C 969	N 283	O 263	${S \over 2}$	0	0	0





• Molecule 7 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
7	Е	180	Total 1468	C 938	N 267	O 259	$\frac{S}{4}$	0	0	0

• Molecule 8 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
8	F	173	Total 1319	C 839	N 245	0 234	S 1	0	0	0

• Molecule 9 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
9	G	148	Total 1156	С 737	N 204	0 214	S 1	0	0	0

• Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
10	Н	138	Total 1103	С 712	N 206	0 182	${ m S} { m 3}$	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Н	24	VAL	MET	$\operatorname{conflict}$	UNP Q72IN1

• Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
11	Ι	122	Total 932	C 587	N 171	0 170	${S \atop 4}$	0	0	0

• Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
12	J	146	Total	С	N	0	S	0	0	0
			1114	692	227	193	2			

• Molecule 13 is a protein called 50S ribosomal protein L16.



Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
13	K	137	Total 1089	C 698	N 207	O 177	${ m S} 7$	0	0	0

• Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
14	L	118	Total 968	C 604	N 203	O 160	S 1	0	0	0

• Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues		Ato	ms		ZeroOcc	AltConf	Trace
15	М	106	Total 846	С 534	N 168	0 144	0	0	0

• Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues		At	$\mathbf{oms}$		ZeroOcc	AltConf	Trace	
16	Ν	137	Total 1143	C 713	N 234	0 195	S 1	0	0	0

• Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
17	О	117	Total 964	C 610	N 202	O 151	S 1	0	0	0

• Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
18	Р	101	Total 779	$\begin{array}{c} \mathrm{C} \\ 501 \end{array}$	N 142	0 135	S 1	0	0	0

• Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
19	Q	109	Total 868	С 547	N 170	O 150	S 1	0	0	0

• Molecule 20 is a protein called 50S ribosomal protein L23.



$\operatorname{Mol}$	Chain	Residues		Ato	$\mathbf{ms}$		ZeroOcc	AltConf	Trace
20	R	92	Total 725	C 471	N 131	O 123	0	0	0

• Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
21	S	103	Total 793	C 510	N 151	O 126	${ m S}{ m 6}$	0	0	0

• Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
22	Т	185	Total 1475	C 941	N 262	O 269	${ m S} { m 3}$	0	0	0

• Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
23	U	76	Total 605	C 376	N 126	0 102	S 1	0	0	0

• Molecule 24 is a protein called LSU ribosomal protein L28P.

Mol	Chain	Residues		Ato	ms		ZeroOcc	AltConf	Trace
24	V	88	Total 694	$\begin{array}{c} \mathrm{C} \\ 435 \end{array}$	N 141	0 118	0	0	0

• Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
25	W	62	Total 520	C 325	N 102	O 91	${ m S} { m 2}$	0	0	0

• Molecule 26 is a protein called LSU ribosomal protein L30P.

Mol	Chain	Residues		Ato	$\mathbf{ms}$			ZeroOcc	AltConf	Trace
26	Х	60	Total 477	C 303	N 91	O 82	S 1	0	0	0

• Molecule 27 is a protein called 50S ribosomal protein L32.



Mol	Chain	Residues		Ato	$\mathbf{ms}$			ZeroOcc	AltConf	Trace
27	Y	56	Total 436	C 275	N 84	0 72	${f S}{5}$	0	0	0

• Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	Trace
28	Z	48	Total 418	C 257	N 104	O 55	${S \over 2}$	0	0	0

• Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
29	a	63	Total 507	C 326	N 101	0 78	${ m S} { m 2}$	0	0	0

• Molecule 30 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues		Atc	$\mathbf{ms}$			ZeroOcc	AltConf	Trace
30	b	35	Total 294	C 181	N 66	0 44	${ m S} { m 3}$	0	0	0

• Molecule 31 is a RNA chain called 16S RNA.

Mol	Chain	Residues		I	Atoms			ZeroOcc	AltConf	Trace
31	У	1514	Total 32546	C 14494	N 6022	O 10517	Р 1513	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
У	466	G	С	conflict	$GB \ 155076$

• Molecule 32 is a RNA chain called P-site tRNAfMET.

Mol	Chain	Residues		A	toms			ZeroOcc	AltConf	Trace
32	Z	77	Total 1639	C 732	N 297	0 534	Р 76	0	0	0

• Molecule 33 is a RNA chain called E-site tRNA.



Mol	Chain	Residues		$\mathbf{A}^{\dagger}$	toms			ZeroOcc	AltConf	Trace
33	2	76	Total 1621	C 725	N 293	O 528	Р 75	0	0	0

• Molecule 34 is a RNA chain called MRNA.

Mol	Chain	Residues		At	$\mathbf{oms}$			ZeroOcc	AltConf	Trace
34	3	18	Total 390	C 176	N 80	0 117	Р 17	0	0	0

• Molecule 35 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
35	с	234	Total 1900	C 1213	N 341	0 341	${ m S}{ m 5}$	0	0	0

• Molecule 36 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
36	d	206	Total 1612	C 1016	N 314	0 281	S 1	0	0	0

• Molecule 37 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
37	е	208	Total 1703	C 1066	N 339	0 291	${f S}{7}$	0	0	0

• Molecule 38 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
38	f	150	Total 1146	С 724	N 217	0 201	$\frac{S}{4}$	0	0	0

• Molecule 39 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
39	g	101	Total 843	C 531	N 155	0 154	${ m S} { m 3}$	0	0	0

• Molecule 40 is a protein called 30S ribosomal protein S7.



Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
40	h	155	Total 1257	C 781	N 252	O 218	S 6	0	0	0

• Molecule 41 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
41	i	138	Total 1116	C 705	N 215	0 193	${ m S} { m 3}$	0	0	0

• Molecule 42 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues		Ato	ms		ZeroOcc	AltConf	Trace
42	j	127	Total 1011	C 639	N 198	0 174	0	0	0

• Molecule 43 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
43	k	98	Total 794	C 499	N 156	0 138	S 1	0	0	0

• Molecule 44 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
44	1	116	Total 864	$\begin{array}{c} \mathrm{C} \\ 537 \end{array}$	N 164	O 160	${ m S} { m 3}$	0	0	0

• Molecule 45 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
45	m	124	Total 970	C 611	N 195	O 163	S 1	0	0	0

• Molecule 46 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
46	n	125	Total 997	C 617	N 207	0 171	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0	0

• Molecule 47 is a protein called 30S ribosomal protein S14 type Z.



Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	Trace
47	0	60	Total 492	C 312	N 104	0 72	$\frac{S}{4}$	0	0	0

• Molecule 48 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
48	р	88	Total 734	C 459	N 147	O 126	${ m S} { m 2}$	0	0	0

• Molecule 49 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
49	q	83	Total 700	C 443	N 139	0 117	S 1	0	0	0

• Molecule 50 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
50	r	104	Total 857	С 547	N 161	0 147	${S \over 2}$	0	0	0

• Molecule 51 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues		Ato	ms		ZeroOcc	AltConf	Trace
51	s	81	Total 668	C 423	N 135	O 110	0	0	0

• Molecule 52 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
52	t	80	Total 647	C 414	N 119	0 112	${S \over 2}$	0	0	0

• Molecule 53 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
53	u	99	Total 762	C 469	N 162	0 129	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0	0

• Molecule 54 is a protein called 30S ribosomal protein Thx.



Mol	Chain	Residues		Aton	ıs		ZeroOcc	AltConf	Trace
54	v	24	Total 208	C 128	N 50	O 30	0	0	0



## 3 Residue-property plots (i)

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



• Molecule 1: 23S LARGE SUBUNIT RIBOSOMAL RNA



U963	C964 C965	<b>G966</b>	(197.7	A973	G974A	G975	C976	1997	A980	A981	C982 A983		0000 0000	A330 C991	C992	6993	A996	<b>G</b> 997	C1006	C1007	C1008 A1009	A1010	G1011	01012 C1013	U1014	G1016	G1017	A1020	G1022	01023 G1024	G1025	07010	01033 01034		G1042 C1043	G1044	A1046	61047	A1054
G1059	U1060 U1061	G1062	A1067	G1068	A1069 A1070	G1071	C1072	C1079	C1080	000 711	01083	G1087	A1088	60015	A1095	A1096 111097	A1098	G1099	A1111	G1112	G115	C1116	G1117	A1126	0.110	U1130	G1131 A1132	U1133	G1136 G1136	G1139	C1140	01141 C1142	A1142B A1143	G1144	A1148			A1155 A1156	G1157
C1161	C1166		G1170 G1171		01175 C1176	A1177	C1178	C1179 C1180	C1181	A1182	61183	G1186	G1187 11180	00110	G1191	A 1 1 94	G1195	C1196 C1197	U1198	U1199	C1200	C1202	G1203	A1204 U1205	1200 1200	G1209	A1210 U1211	G1212	A1220	C1221 C1221A	1000 1000 1000	01224	G1227 G1228	G1229	A1237	G1238	01240	G1244	A1247
G1248	01249 G1250	C1251	G1252 A1253		G1256	A1265	G1266	0126/	G1271	A1272	012/3 A1274	A1275	A1276	A1278	G1279	61280	U1288	C1289	C1295	G1296	C1297 C1298	G1299	U1300	A1301 A1302	C130E		G1310	U1313	C1320	A1321	G1325	07250	U1329	G1339	<mark>U1340</mark> U1341	A1342		G134/ G1348	A1349
G1356	A1359	A1360	G1361 C1362		A1365 A1366	A1367	G1368	61369	A1378	A1379	A1384	G1385	4 1 3 0 H	CACTW	C1398	C1404	U1405	61416		G1418	A1419 111420		G1426	A 1427 C 1428	41424	G1435	G1436 C1437	U1438	A1444B	C1445	G1448	A 1446b G 1449	C1450 C1451	A1453	U1454 G1455	2 2 2 2	G1459	A1460 G1461	C1467
	A1471 A1472	G1473	C1474	G1478	G1479 C1480	U1481	G1483	G1484 G1485	A1486	G1487	01488 01489	A1490	G1491	A1496	U1497	C1498	G1500	C1501	20010	C1506	A1508 A1509	A1510		01515 G1517	C1518	U1520	G1521 G1522	100 100	U1535	A1536 C1537	G1538 61538	G1540	A1543	C1544	A1545 A1546	C1546B		61555 6	A1558 G1559
G1560	A1567	G1568	A1569 A1570		01576 C1577	U1578	A1579	A1580 G1581	C1582	A1583	C1585 A1586		U1590	C1592	G1593	G1594 G1595	A1596	1500	C1600		A1603	C1607	A1608	A1609 A1610	C1610	A1614	C1615 A1616	C1617	G1619	C1625	G1626	G1628	C1630B		G1633 • A1634 •	G1635		01639 C1640	A1641 G1642
	C1646 G1647	C1648	A1654		A1664	G1666		A1669 C1670	U1671	C1672	01673 G1674		G1678	U1680	G1681	61682	U1688	111607	U1693	C1694	61699 61699	A1700		61/03	G1707	C1712	01716 G1717	G1718	G1731	A1/32 G1733	C1734	C1741	C1742 G1743	G1746	G1747 G1748		A1755	G1756 U1757	G1758 A1759
A1760	C1761 A1762	G1763	G1764	A1773	C1774	G1776	01777	A1780	C1781	C1782	A1785	A1786	A1787	G1792	2	C1800 G1801	A1802	C1806	G1807	U1808	A1809	G1811	A1812	A1815	G1816 C1817	U1818	A1819 U1820	A1821	G1823	G1824 A1825	4	A 1023	C1836 C1837	C1838	G1839	C1843	A1847	G1858	A1859
G1863	01864 G1869		A1872 G1878	C1879	A1 885	C1886	C1887	GT 888 A1 889		U1 898	G1899 A1900		G1903	G1906		A1912 A1913	C1914	U1915 A1916	OTETH	G1929	G1930	G1935	A1936	A1937 A1938	U1939	01 <mark>944</mark>	U1955	U1956	A1960	U1963	G1964 C1065	C1305 A1966	C1967 C1968	A1969	A1970 A1971	A1972	A1977	C1982	C1 983
G1987	C1988 G1989	C1990	U1991 G1992	U1993	C1 007	G1998		A2001 G2002		G2010	G2012	A2013	A2014	A2020		62023	c2026	40031	G2032	A2033	02034 02035		C2040	02041 A2042	C2043	C2050	A2051 G2052		G2056	A2057 A2058	A2059	A2060 G2061	A2062 C2063		C2066 G2067	U2068		U2076 A2077	G2080
	62087	U2092	G2093	<mark>U2096</mark>		G2100		G21110 C2111	G2112		G2116 A2117	U2118	A2119	G2120 G2121	U2122	G2123	G2125	A2126	C2128	C2129	U2130 C2131	U2132	G2133	C2136	C2137		C2145	G2157	G2159	G2160 C2161	G2162	A2169	A2170 A2171	U2172	A2173 C2174	C2175	C2177	C2178 C2179	U2180 G2181
-	C2188 U2189	G2190	G2191 G2192	G2193	G2194 C2195		A2199	C2205	G2211	A2212	02213 G2215	G2216	G2217	G2219 G2219	G2224	A2225 C2226		G2238 G2738		U2243	C2248		G2251	U2257	C2258	C2260	C2264		6077W	A2274 C2275	G2276	C2283	42287	A2288	G2289 G2290			C2297	G2304 A2305









 $\bullet$  Molecule 8: 50S ribosomal protein L6

![](_page_16_Picture_5.jpeg)

![](_page_17_Figure_3.jpeg)

![](_page_17_Picture_4.jpeg)

![](_page_18_Figure_3.jpeg)

#### A115 A116 Q117 G118

![](_page_19_Figure_4.jpeg)

![](_page_19_Picture_5.jpeg)

![](_page_20_Figure_3.jpeg)

• Molecule 29: 50S ribosomal protein L35

![](_page_20_Picture_5.jpeg)

![](_page_21_Figure_2.jpeg)

![](_page_21_Figure_3.jpeg)

![](_page_21_Picture_4.jpeg)

![](_page_22_Figure_2.jpeg)

![](_page_22_Picture_4.jpeg)

![](_page_23_Figure_3.jpeg)

![](_page_24_Figure_3.jpeg)

![](_page_24_Picture_4.jpeg)

![](_page_25_Figure_3.jpeg)

# 194 MET 195 P2 190 V10 114 V110 114 V111 115 V111 116 V111 117 V111 114 V111

• Molecule 51: 30S ribosomal protein S18

Chain s:	69%		22%	• 8%	
MET SER THR LVYS ALA ALA ALA KIO KIO G13 G13	R14 15 125 125 125 125 123 133 133 133 133 133 133 133 133 133	147 153 859 859 463 176 176 182 182	K88		
• Molecule 52: 30	0S ribosomal protein	S19			
Chain t:	46%	34%	5%	14%	
MET K6 K7 K7 K7 K7 K7 K7 K7 K7 K7 K7 K7 K7 K7	K28 K28 K28 K28 K32 K32 K32 K33 K33 K33 K33 K33 K33 K33	E43 444 445 446 446 149 149 152 152 155 155 155	V58 P59 V60 V61 162 T62 E64 M65	M66 V67 K70 L71	P76 T77 R78 R81
GLY HIS GLY CLY CLV CLU ALA ALA ALA ALA THR LYS LYS LYS					
• Molecule 53: 30	0S ribosomal protein	S20			
Chain u:	71%		22%	• 7%	-
MET ALA ALA GLN GLN LYS FRO FRO FRO IJO NG NG NG NG NG NG	L20 K21 K21 K22 R23 R23 R23 R24 K44 C41 C43 C45 C47 C47 C47 C47	449 850 851 851 851 851 153 153 153 153 171 171 177 177 177	R79 190 191 191 192 192 893 €93	A97 P98 1100 A106	
• Molecule 54: 30	0S ribosomal protein	Thx			

![](_page_26_Picture_6.jpeg)

![](_page_26_Picture_7.jpeg)

## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants	507.21Å 507.21Å 692.51Å	Deperitor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
$\mathbf{B}_{\mathrm{ascolution}}\left(\mathring{A}\right)$	30.00 - 3.83	Depositor
Resolution (A)	78.70 - 3.70	EDS
% Data completeness	81.7 (30.00-3.83)	Depositor
(in resolution range)	68.4(78.70-3.70)	EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.43 (at 3.67 \text{\AA})$	Xtriage
Refinement program	REFMAC $5.2.0019$ , CNS	Depositor
B B.	0.327 , $0.351$	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.340 , $0.360$	DCC
$R_{free}$ test set	10300 reflections $(2.90%)$	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.5	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.07 , -110.0	EDS
L-test for $twinning^2$	$<  L  > = 0.22, < L^2 > = 0.07$	Xtriage
	0.267  for  -1/2 *h+1/2 *k-1/2 *l, 1/2 *h-1/2 *k-1/2 *k-1/2 *h-1/2 *k-1/2 *h-1/2 *	
Estimated twinning fraction	1/2*l,-h-k	Xtriage
0	$0.260 \text{ for } -1/2^{\text{h}-1}/2^{\text{k}+1}/2^{\text{l},-1}/2^{\text{h}-1}/2^{\text{k}-1}$	
E.E. correlation	1/2 <sup>-1</sup> ,n-k	FDG
$\frac{\Gamma_{o}, \Gamma_{c} \text{ correlation}}{\text{Total number of stores}}$	0.09	
Access D all stores ( <sup>8</sup> 2)	14(12)	
Average B, all atoms $(A^2)$	1.0	WWPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 1.08% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

![](_page_27_Picture_8.jpeg)

<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 5 Model quality (i)

#### 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 7MG, 5MC, PSU, 2MG, MA6, M2G  $\,$ 

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).

Mal	Chain	B	ond lengths	I	Bond angles
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	W	1.00	42/69679~(0.1%)	1.03	92/108779~(0.1%)
2	Х	0.65	1/2878~(0.0%)	0.90	1/4490~(0.0%)
3	А	0.53	0/1015	0.63	0/1369
4	В	0.53	0/2165	0.70	0/2919
5	С	0.56	0/1574	0.69	0/2125
6	D	0.58	0/1551	0.69	0/2101
7	Ε	0.58	0/1492	0.72	1/2006~(0.0%)
8	F	0.56	0/1345	0.70	0/1819
9	G	0.51	0/1171	0.70	0/1583
10	Н	0.54	0/1130	0.71	1/1525~(0.1%)
11	Ι	0.57	0/942	0.74	1/1268~(0.1%)
12	J	0.57	0/1131	0.76	1/1504~(0.1%)
13	Κ	0.58	0/1110	0.74	1/1483~(0.1%)
14	L	0.49	0/982	0.69	0/1312
15	М	0.51	0/856	0.63	0/1138
16	Ν	0.56	0/1157	0.72	0/1544
17	0	0.53	0/982	0.64	0/1306
18	Р	0.58	0/790	0.69	0/1057
19	Q	0.51	0/878	0.74	1/1179~(0.1%)
20	R	0.60	0/739	0.75	0/993
21	S	0.61	0/806	0.70	0/1074
22	Т	0.54	0/1507	0.66	0/2045
23	U	0.56	0/613	0.75	0/816
24	V	0.64	0/701	0.71	0/932
25	W	0.53	0/522	0.75	0/690
26	Х	0.51	0/482	0.66	0/646
27	Y	0.53	0/449	0.69	0/606
28	Z	0.52	0/426	0.65	0/561
29	a	0.56	0/515	0.70	0/679
30	b	0.60	0/297	0.63	0/392
31	у	0.72	23/36178~(0.1%)	0.93	44/56463~(0.1%)
32	Z	0.62	0/1831	0.88	0/2853

![](_page_28_Picture_8.jpeg)

Mal	Chain	B	ond lengths	I	Bond angles
	Unain	RMSZ	# Z  > 5	RMSZ	# Z  > 5
33	2	0.65	0/1791	0.85	0/2791
34	3	0.63	0/439	0.90	0/684
35	с	0.56	0/1935	0.67	0/2609
36	d	0.51	0/1636	0.68	0/2205
37	е	0.55	0/1733	0.68	1/2318~(0.0%)
38	f	0.60	0/1162	0.68	0/1564
39	g	0.55	0/856	0.70	0/1154
40	h	0.54	0/1276	0.63	0/1709
41	i	0.51	0/1136	0.68	0/1527
42	j	0.58	0/1029	0.66	0/1378
43	k	0.59	0/807	0.66	0/1085
44	1	0.58	0/879	0.64	0/1187
45	m	0.55	0/986	0.75	0/1320
46	n	0.54	0/1008	0.68	0/1347
47	0	0.52	0/501	0.67	0/664
48	р	0.50	0/745	0.64	0/992
49	q	0.57	0/716	0.70	0/963
50	r	0.55	0/870	0.71	0/1159
51	s	0.60	0/675	0.67	0/894
52	t	0.59	0/661	0.68	1/890~(0.1%)
53	u	0.46	0/764	0.65	0/1006
54	V	0.58	0/212	0.60	0/277
All	All	0.81	66/159711~(0.0%)	0.92	145/238980~(0.1%)

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
1	W	41	С	O3'-P	43.37	2.13	1.61
1	W	1506	С	O3'-P	40.09	2.09	1.61
1	W	489	G	O3'-P	39.72	2.08	1.61
1	W	1448(B)	А	O3'-P	38.61	2.07	1.61
1	W	436	С	O3'-P	36.62	2.05	1.61
1	W	554	U	O3'-P	36.54	2.04	1.61
1	W	1743	G	O3'-P	36.44	2.04	1.61
1	W	1712	С	O3'-P	36.33	2.04	1.61
1	W	2213	U	O3'-P	35.61	2.03	1.61
1	W	366(B)	С	O3'-P	35.53	2.03	1.61
1	W	2712(B)	А	O3'-P	35.29	2.03	1.61
1	W	890	А	O3'-P	34.85	2.02	1.61
1	W	926	А	O3'-P	34.47	2.02	1.61
1	W	155	С	O3'-P	34.19	2.02	1.61
1	W	1583	А	O3'-P	33.94	2.01	1.61

![](_page_29_Picture_7.jpeg)

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	W	99	U	O3'-P	33.39	2.01	1.61
1	W	1718	G	O3'-P	33.29	2.01	1.61
1	W	1481	U	O3'-P	31.86	1.99	1.61
1	W	1451	С	O3'-P	31.83	1.99	1.61
1	W	1735	U	O3'-P	31.62	1.99	1.61
1	W	537	С	O3'-P	31.45	1.98	1.61
1	W	1864	U	O3'-P	30.27	1.97	1.61
1	W	1171	G	O3'-P	30.16	1.97	1.61
1	W	1546(B)	С	O3'-P	29.62	1.96	1.61
1	W	1630(B)	С	O3'-P	29.10	1.96	1.61
1	W	1872	А	O3'-P	28.59	1.95	1.61
1	W	1142(B)	А	O3'-P	28.49	1.95	1.61
1	W	2219	G	O3'-P	28.38	1.95	1.61
1	W	1221(A)	С	O3'-P	27.85	1.94	1.61
1	W	165	U	O3'-P	27.37	1.94	1.61
1	W	1444(B)	А	O3'-P	26.83	1.93	1.61
1	W	1133	U	O3'-P	25.03	1.91	1.61
31	У	201	С	O3'-P	23.92	1.89	1.61
1	W	2199	А	O3'-P	21.55	1.87	1.61
31	у	97	U	O3'-P	18.57	1.83	1.61
1	W	2799	А	O3'-P	17.20	1.81	1.61
1	W	2746	U	O5'-C5'	16.23	1.70	1.44
1	W	2795	G	O3'-P	15.55	1.79	1.61
31	у	99	С	O3'-P	15.40	1.79	1.61
31	У	103(C)	G	O3'-P	15.38	1.79	1.61
31	У	1455	G	O3'-P	14.53	1.78	1.61
31	У	843	U	O3'-P	13.63	1.77	1.61
31	У	136(B)	С	O3'-P	13.10	1.76	1.61
31	У	458	С	O3'-P	13.00	1.76	1.61
31	У	1498	U	C4-O4	12.92	1.33	1.23
31	У	102(C)	С	O3'-P	12.51	1.76	1.61
1	W	2746	U	O3'-P	11.80	1.75	1.61
31	У	838	G	O3'-P	11.41	1.74	1.61
1	W	2889	C	03'-P	11.28	1.74	1.61
31	У	93	U	O3'-P	9.74	1.72	1.61
31	У	1167	A	O3'-P	8.96	1.72	1.61
1	W	2747	G	P-O5'	8.92	1.68	1.59
31	У	1402	C	P-O5'	8.88	1.68	1.59
1	W	2746	U	P-05'	8.37	1.68	1.59
1	W	2722	G	O5'-C5'	7.90	1.57	1.44
31	У	1402	С	O5'-C5'	7.66	1.56	1.44
31	У	99	C	P-05'	7.37	1.67	1.59

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![](_page_30_Picture_6.jpeg)

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
31	У	1402	С	C4-N4	7.28	1.40	1.33
31	У	69	G	O3'-P	7.14	1.69	1.61
1	W	2720	U	O5'-C5'	6.96	1.55	1.44
2	Х	29	А	P-O5'	5.49	1.65	1.59
31	У	97	U	O5'-C5'	5.49	1.53	1.44
31	У	449	С	O5'-C5'	5.45	1.53	1.44
31	У	162	А	O5'-C5'	5.27	1.52	1.44
31	У	1114	С	O5'-C5'	5.08	1.52	1.44
31	у	37	U	O5'-C5'	5.02	1.52	1.44

Continued from previous page...

All (145) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	W	2712(B)	А	P-O3'-C3'	-23.05	92.04	119.70
1	W	489	G	P-O3'-C3'	-18.72	97.23	119.70
31	У	97	U	P-O3'-C3'	-16.92	99.40	119.70
1	W	41	С	P-O3'-C3'	-15.29	101.35	119.70
1	W	1712	С	P-O3'-C3'	-15.07	101.61	119.70
31	У	99	С	P-O3'-C3'	-15.02	101.68	119.70
1	W	155	С	P-O3'-C3'	-13.31	103.73	119.70
1	W	537	С	P-O3'-C3'	-12.70	104.46	119.70
1	W	1718	G	P-O3'-C3'	-12.30	104.94	119.70
1	W	2746	U	P-O5'-C5'	-11.99	101.71	120.90
31	у	136(B)	С	P-O3'-C3'	-11.73	105.63	119.70
1	W	436	С	P-O3'-C3'	-11.65	105.72	119.70
1	W	99	U	P-O3'-C3'	-11.53	105.86	119.70
1	W	2393	А	N9-C1'-C2'	-11.49	99.07	114.00
31	У	201	С	P-O3'-C3'	-10.95	106.56	119.70
31	У	93	U	P-O3'-C3'	-10.73	106.83	119.70
1	W	1735	U	P-O3'-C3'	-10.67	106.90	119.70
1	W	1506	С	P-O3'-C3'	-10.31	107.32	119.70
1	W	1133	U	P-O3'-C3'	-10.18	107.49	119.70
31	У	838	G	P-O3'-C3'	-10.06	107.63	119.70
1	W	890	А	P-O3'-C3'	-9.59	108.19	119.70
1	W	1221(A)	С	P-O3'-C3'	-9.46	108.35	119.70
31	У	1402	С	P-O5'-C5'	-9.20	106.18	120.90
1	W	1743	G	P-O3'-C3'	-9.02	108.88	119.70
1	W	2799	А	O3'-P-O5'	9.00	121.11	104.00
1	W	1448(B)	А	P-O3'-C3'	-8.98	108.92	119.70
31	У	1455	G	OP1-P-O3'	8.80	124.56	105.20
31	У	103(C)	G	P-O3'-C3'	-8.77	109.18	119.70
1	W	2805	G	OP2-P-O3'	8.38	123.62	105.20

![](_page_31_Picture_8.jpeg)

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	$Ideal(^{o})$
1	W	926	A	P-03'-C3'	-8.35	109.69	119.70
1	W	1577	C	N1-C1'-C2'	-8.29	102.88	112.00
1	W	2795	G	P-O3'-C3'	-8.10	109.97	119.70
1	W	1955	U	N1-C1'-C2'	8.07	124.49	114.00
1	W	1822	G	N9-C1'-C2'	-8.05	103.15	112.00
31	у	99	С	OP2-P-O3'	8.05	122.90	105.20
1	W	2795	G	OP2-P-O3'	7.77	122.29	105.20
1	W	2257	U	N1-C1'-C2'	-7.67	103.57	112.00
1	W	2431	U	N1-C1'-C2'	-7.47	103.78	112.00
1	W	2805	G	OP1-P-O3'	-7.41	88.90	105.20
1	W	1863	G	N9-C1'-C2'	-7.38	103.88	112.00
31	у	1401	G	C3'-C2'-C1'	-7.37	95.60	101.50
1	W	1872	А	P-O3'-C3'	-7.29	110.95	119.70
31	у	82	U	P-O3'-C3'	7.22	128.37	119.70
1	W	366(B)	С	P-O3'-C3'	-7.15	111.12	119.70
1	W	458	G	C1'-O4'-C4'	-7.11	104.21	109.90
1	W	1955	U	O4'-C1'-N1	6.93	113.75	108.20
1	W	1187	G	N9-C1'-C2'	6.92	123.00	114.00
31	у	99	С	O3'-P-O5'	-6.86	90.96	104.00
1	W	1059	G	O4'-C1'-N9	6.86	113.69	108.20
1	W	362	U	C3'-C2'-C1'	-6.85	96.02	101.50
31	у	1401	G	P-O3'-C3'	-6.84	111.49	119.70
1	W	1444(B)	А	P-O3'-C3'	-6.80	111.54	119.70
1	W	1451	С	O3'-P-O5'	-6.77	91.14	104.00
31	у	210	U	P-O3'-C3'	6.69	127.73	119.70
1	W	873	G	N9-C1'-C2'	-6.64	104.70	112.00
1	W	2213	U	P-O3'-C3'	-6.62	111.75	119.70
2	Х	21	G	N9-C1'-C2'	-6.58	104.76	112.00
19	Q	51	LEU	CA-CB-CG	6.58	130.43	115.30
1	W	800	А	O4'-C1'-N9	6.53	113.43	108.20
1	W	1171	G	P-O3'-C3'	-6.50	111.90	119.70
31	У	890	G	N9-C1'-C2'	-6.39	104.97	112.00
1	W	1274	А	N9-C1'-C2'	-6.39	104.98	112.00
1	W	1822	G	O4'-C1'-N9	6.38	113.30	108.20
31	у	1498	U	N1-C1'-C2'	6.35	122.26	114.00
31	у	189	U	N1-C1'-C2'	-6.35	105.02	112.00
31	у	93	U	<u>OP2-P-O3'</u>	6.22	118.88	105.20
1	W	1516	U	N1-C1'-C2'	-6.11	105.28	112.00
1	W	458	G	O4'-C1'-N9	6.09	113.07	108.20
31	У	1517	G	<u>C3'-C2'-C1'</u>	-6.07	96.64	101.50
1	W	265	A	N9-C1'-C2'	5.97	$1\overline{21.77}$	114.00
31	У	99	С	P-O5'-C5'	-5.95	$1\overline{11.39}$	120.90

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![](_page_32_Picture_6.jpeg)

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Conti Mal	nuea fron	<i>previous</i>	page	Atoma	7	Observed(0)	Ideal(0)
	Unain	$\mathbf{Res}$	Type	Atoms			10eal(°)
31	У	136(B)	C	0P2-P-03 <sup>7</sup>	5.94	118.28	105.20
31	У	843	U	0PI-P-03'	5.88	118.13	105.20
1	W	828	U 	N1-C1'-C2'	5.87	121.63	114.00
1	W	2885	C	C3'-C2'-C1'	-5.84	96.83	101.50
1	W	1577	C	04'-C1'-N1	5.80	112.84	108.20
31	У	102(C)	C	OP2-P-O3'	5.78	117.92	105.20
1	W	1221(A)	C	OP2-P-O3'	5.78	117.91	105.20
31	У	102(C)	С	O3'-P-O5'	-5.77	93.04	104.00
1	W	362	U	N1-C1'-C2'	-5.77	105.66	112.00
1	W	2746	U	P-O3'-C3'	-5.74	112.81	119.70
31	У	210	U	OP1-P-O3'	-5.74	92.57	105.20
1	W	227	А	P-O3'-C3'	5.74	126.58	119.70
31	У	1498	U	C5-C4-O4	-5.73	122.46	125.90
1	W	1800	С	O4'-C1'-N1	5.73	112.78	108.20
1	W	1615	С	O4'-C1'-N1	5.69	112.75	108.20
31	У	1105	А	N9-C1'-C2'	-5.65	105.78	112.00
31	У	587	G	O4'-C1'-N9	5.63	112.71	108.20
1	W	241	А	O4'-C1'-N9	5.63	112.70	108.20
1	W	271(D)	U	O4'-C1'-N1	5.62	112.70	108.20
52	t	71	LEU	CA-CB-CG	5.62	128.23	115.30
1	W	15	G	N9-C1'-C2'	-5.61	105.83	112.00
31	у	1455	G	O3'-P-O5'	-5.59	93.38	104.00
1	W	70	G	N9-C1'-C2'	5.57	121.24	114.00
1	W	2393	А	O4'-C1'-N9	5.56	112.65	108.20
1	W	1288	U	P-O3'-C3'	5.55	126.36	119.70
31	У	436	С	N1-C1'-C2'	-5.53	105.92	112.00
1	W	2468	G	N9-C1'-C2'	-5.53	105.92	112.00
1	W	913	U	P-O3'-C3'	5.51	126.32	119.70
31	у	1254	С	N1-C1'-C2'	-5.51	105.94	112.00
1	W	99	U	OP1-P-O3'	5.48	117.25	105.20
1	W	2225	А	P-O3'-C3'	5.48	126.27	119.70
1	W	2171	А	N9-C1'-C2'	5.47	121.12	114.00
31	у	69	G	O3'-P-O5'	-5.46	93.63	104.00
1	W	932	G	N9-C1'-C2'	5.46	121.09	114.00
1	W	1626	G	O4'-C1'-N9	5.43	112.54	108.20
12	J	148	LEU	CA-CB-CG	5.42	127.77	115.30
1	W	1898	U	N1-C1'-C2'	5.41	121.03	114.00
1	W	2497	А	P-O3'-C3'	5.36	126.14	119.70
1	W	2171	А	P-O3'-C3'	5.36	126.13	119.70
31	V	210	U	OP2-P-O3'	5.35	116.97	105.20
31	V	468	A	O3'-P-O5'	5.34	114.14	104.00
7	Ē	139	LEU	CA-CB-CG	5.33	127.57	115.30

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![](_page_33_Picture_6.jpeg)

Mol	Chain	$\operatorname{Res}$	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
11	Ι	91	LEU	CA-CB-CG	5.32	127.54	115.30
1	W	933	А	O4'-C1'-N9	5.30	112.44	108.20
31	у	250	А	N9-C1'-C2'	-5.30	106.17	112.00
31	у	1521	G	N9-C1'-C2'	-5.28	106.19	112.00
1	W	448	U	C1'-O4'-C4'	-5.28	105.67	109.90
13	Κ	37	LEU	CA-CB-CG	5.28	127.45	115.30
1	W	270(E)	С	N1-C1'-C2'	5.28	120.86	114.00
1	W	2002	G	O4'-C1'-N9	5.28	112.42	108.20
31	у	1220	G	N9-C1'-C2'	-5.27	106.20	112.00
1	W	2205	С	N1-C1'-C2'	-5.27	106.20	112.00
1	W	739	G	P-O3'-C3'	5.26	126.02	119.70
31	у	1401	G	N9-C1'-C2'	-5.24	106.24	112.00
1	W	1775	U	C3'-C2'-C1'	-5.24	97.31	101.50
31	у	960	U	N1-C1'-C2'	5.24	120.81	114.00
31	у	1498	U	N1-C2-N3	5.21	118.03	114.90
31	у	659	U	C3'-C2'-C1'	-5.21	97.34	101.50
31	у	1498	U	C2-N3-C4	-5.20	123.88	127.00
1	W	1247	А	C1'-O4'-C4'	-5.19	105.75	109.90
1	W	299	А	O4'-C1'-N9	5.18	112.34	108.20
1	W	1266	G	P-O3'-C3'	5.18	125.91	119.70
10	Н	38	LEU	CA-CB-CG	5.17	127.20	115.30
37	е	19	LEU	CA-CB-CG	5.15	127.14	115.30
1	W	520	G	C3'-C2'-C1'	-5.15	97.38	101.50
1	W	1426	G	N9-C1'-C2'	5.13	120.68	114.00
1	W	554	U	P-O3'-C3'	-5.13	113.54	119.70
1	W	1812	А	C4'-C3'-C2'	-5.10	97.50	102.60
1	W	204	А	C3'-C2'-C1'	5.09	105.57	101.50
1	W	1356	G	O4'-C1'-N9	5.09	112.27	108.20
31	у	1402	С	C3'-C2'-C1'	5.06	105.55	101.50
1	W	1534	G	C3'-C2'-C1'	-5.04	97.47	101.50
1	W	457	А	N9-C1'-C2'	5.02	120.53	114.00
1	W	2848	G	O4'-C1'-N9	5.01	112.20	108.20

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There are no chirality outliers.

There are no planarity outliers.

#### 5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

![](_page_34_Picture_9.jpeg)

#### 5.3 Torsion angles (i)

#### 5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	Favoured Allowed Outli		Percentiles	
3	А	123/229~(54%)	72~(58%)	31~(25%)	20~(16%)	0 3	
4	В	270/276~(98%)	134~(50%)	64~(24%)	72~(27%)	0 0	
5	С	199/206~(97%)	99~(50%)	47 (24%)	53~(27%)	0 0	
6	D	192/205~(94%)	91 (47%)	45~(23%)	56~(29%)	0 0	
7	Ε	178/182~(98%)	97~(54%)	55 (31%)	26~(15%)	0 4	
8	F	171/180~(95%)	90~(53%)	40 (23%)	41 (24%)	0 1	
9	G	146/148~(99%)	83~(57%)	35~(24%)	28~(19%)	0 2	
10	Н	136/140~(97%)	62 (46%)	45 (33%)	29~(21%)	0 1	
11	Ι	120/122~(98%)	62~(52%)	24 (20%)	34 (28%)	0 0	
12	J	144/150~(96%)	63 (44%)	46 (32%)	35 (24%)	0 1	
13	К	135/141~(96%)	56 (42%)	41 (30%)	38~(28%)	0 0	
14	L	116/118 (98%)	64 (55%)	30 (26%)	22~(19%)	0 2	
15	М	104/112~(93%)	58~(56%)	22 (21%)	24 (23%)	0 1	
16	Ν	135/146~(92%)	56 (42%)	40 (30%)	39~(29%)	0 0	
17	Ο	115/118~(98%)	66~(57%)	28 (24%)	21~(18%)	0 2	
18	Р	99/101~(98%)	39~(39%)	28~(28%)	32~(32%)	0	
19	Q	107/113~(95%)	64 (60%)	23~(22%)	20~(19%)	0 2	
20	R	90/96~(94%)	29~(32%)	36 (40%)	25~(28%)	0 0	
21	S	101/110~(92%)	28 (28%)	31 (31%)	42 (42%)	0 0	
22	Т	183/206~(89%)	115 (63%)	45 (25%)	23~(13%)	0 5	
23	U	74/85~(87%)	31 (42%)	21 (28%)	22 (30%)	0	
24	V	86/98~(88%)	41 (48%)	29 (34%)	16 (19%)	0 2	
25	W	60/72~(83%)	33 (55%)	11 (18%)	16 (27%)	0 0	
26	Х	58/60~(97%)	31 (53%)	20 (34%)	7 (12%)	0 6	
27	Y	54/60~(90%)	27 (50%)	16 (30%)	11 (20%)	0 2	

![](_page_35_Picture_9.jpeg)
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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Pere	centiles
28	Z	46/49~(94%)	31 (67%)	10 (22%)	5 (11%)	C	8
29	a	61/65~(94%)	28 (46%)	20 (33%)	13 (21%)	C	1
30	b	33/37~(89%)	16 (48%)	10 (30%)	7 (21%)	C	2
35	с	232/256~(91%)	142 (61%)	59~(25%)	31~(13%)	C	4
36	d	204/239~(85%)	102 (50%)	60~(29%)	42 (21%)	C	2
37	е	206/209~(99%)	120 (58%)	60~(29%)	26~(13%)	C	5
38	f	148/162~(91%)	102 (69%)	32~(22%)	14 (10%)	0	11
39	g	99/101~(98%)	72 (73%)	19~(19%)	8 (8%)	1	14
40	h	153/156~(98%)	96 (63%)	30 (20%)	27~(18%)	C	3
41	i	136/138~(99%)	84 (62%)	33~(24%)	19 (14%)	C	4
42	j	125/128~(98%)	81 (65%)	29~(23%)	15~(12%)	C	6
43	k	96/105~(91%)	55~(57%)	25~(26%)	16 (17%)	C	3
44	1	114/129~(88%)	74 (65%)	28 (25%)	12 (10%)	C	9
45	m	122/132~(92%)	67~(55%)	35~(29%)	20 (16%)	C	3
46	n	123/126~(98%)	70 (57%)	35~(28%)	18 (15%)	C	4
47	О	58/61~(95%)	30~(52%)	16 (28%)	12 (21%)	C	2
48	р	86/89~(97%)	51 (59%)	24 (28%)	11 (13%)	C	5
49	q	81/88~(92%)	34 (42%)	25~(31%)	22~(27%)	C	0
50	r	102/105~(97%)	54 (53%)	24 (24%)	24 (24%)	C	1
51	s	79/88~(90%)	45 (57%)	21 (27%)	13 (16%)	C	3
52	$\mathbf{t}$	78/93~(84%)	30 (38%)	26 (33%)	22 (28%)	C	0
53	u	97/106~(92%)	47 (48%)	35~(36%)	15 (16%)	C	4
54	V	22/27~(82%)	8 (36%)	6 (27%)	8 (36%)	C	0
All	All	5697/6163~(92%)	3030 (53%)	1515 (27%)	1152 (20%)	C	2

All (1152) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	А	8	TYR
3	А	16	ASP
3	А	63	VAL
3	А	176	VAL
3	А	179	ALA
3	А	180	SER



Mol	Chain	Res	Type
3	А	209	PHE
4	В	3	VAL
4	В	6	PHE
4	В	15	PHE
4	В	21	PHE
4	В	36	PRO
4	В	39	LYS
4	В	44	ASN
4	В	59	LYS
4	В	69	ARG
4	В	83	GLU
4	В	91	ARG
4	В	105	ILE
4	В	138	VAL
4	В	149	PRO
4	В	156	ALA
4	В	196	VAL
4	В	206	LEU
4	В	209	ALA
4	В	227	ASN
4	В	228	PRO
4	В	235	GLY
4	В	239	ARG
4	В	259	THR
4	В	262	ARG
4	В	263	ARG
5	С	35	GLN
5	С	51	PHE
5	С	54	GLN
5	С	65	GLY
5	С	67	PHE
5	С	73	GLU
5	С	77	ILE
5	С	82	ARG
5	С	104	VAL
5	С	121	ASN
5	С	122	PHE
5	С	128	SER
5	С	143	ASN
5	С	144	ARG
5	С	149	ARG
5	С	178	GLU



Mol	Chain	Res	Type
5	С	189	PRO
6	D	17	ALA
6	D	18	ASP
6	D	23	ILE
6	D	38	LYS
6	D	48	THR
6	D	54	TYR
6	D	58	LYS
6	D	59	ILE
6	D	68	ALA
6	D	87	PRO
6	D	120	LEU
6	D	128	ASN
6	D	146	SER
6	D	172	ALA
6	D	176	LEU
6	D	196	VAL
7	Е	13	GLU
7	Е	26	GLN
7	Е	29	TRP
7	Е	78	SER
7	Е	79	ASN
7	Е	82	LEU
7	Е	84	LYS
7	Е	87	PRO
7	Е	88	ILE
7	Е	95	ARG
7	Е	163	ALA
7	Е	181	ARG
8	F	10	PRO
8	F	40	GLU
8	F	52	VAL
8	F	55	PRO
8	F	58	GLU
8	F	71	LEU
8	F	99	VAL
8	F	101	ARG
8	F	109	PHE
8	F	157	TYR
8	F	173	PRO
8	F	178	ALA
9	G	8	PRO



Mol	Chain	Res	Type
9	G	26	ALA
9	G	29	TYR
9	G	38	LEU
9	G	82	ARG
9	G	94	ALA
9	G	122	GLU
9	G	125	GLU
9	G	132	PRO
9	G	138	ILE
10	Н	26	THR
10	Н	67	PRO
10	Н	102	PRO
10	Η	108	ILE
10	Н	110	LEU
10	Η	146	TYR
10	Н	147	ALA
10	Н	153	HIS
11	Ι	5	GLN
11	Ι	51	ALA
11	Ι	52	VAL
11	Ι	54	GLU
11	Ι	60	ALA
11	Ι	63	VAL
11	Ι	75	SER
11	Ι	85	VAL
11	Ι	90	GLN
11	Ι	91	LEU
11	Ι	115	VAL
12	J	12	ALA
12	J	17	LYS
12	J	33	ARG
12	J	35	HIS
12	J	45	LEU
$1\overline{2}$	J	52	GLU
12	J	71	VAL
$1\overline{2}$	J	90	ARG
12	J	106	LEU
12	J	119	GLU
$1\overline{2}$	J	124	LYS
12	J	148	LEU
13	K	3	MET
13	K	4	PRO



Mol	Chain	Res	Type
13	K	21	THR
13	K	25	ASP
13	К	27	VAL
13	K	31	ASP
13	K	38	GLU
13	K	68	ILE
13	K	73	PRO
13	K	79	LEU
13	K	80	GLU
13	K	81	VAL
13	K	83	MET
13	K	85	LYS
13	K	108	GLY
13	K	120	ILE
13	K	127	ILE
13	K	133	ARG
14	L	2	ARG
14	L	5	LYS
14	L	12	ARG
14	L	37	THR
14	L	45	ARG
14	L	60	LEU
14	L	62	ALA
14	L	95	THR
14	L	102	GLU
14	L	104	ARG
14	L	117	VAL
15	М	8	GLU
15	М	9	ARG
15	М	10	ARG
15	М	12	PHE
15	М	32	LEU
15	М	35	ILE
16	Ν	12	SER
16	Ν	18	ASP
16	N	28	VAL
16	N	30	VAL
16	Ν	33	LYS
16	N	42	ILE
16	Ν	45	PHE
16	N	74	ARG
16	N	83	ILE



Mol	Chain	Res	Type
16	N	96	ARG
16	N	101	PHE
16	N	107	ASP
16	N	135	VAL
17	0	6	THR
17	0	22	LYS
17	0	25	TRP
17	0	76	TYR
17	0	90	VAL
17	0	92	ARG
17	0	104	GLN
17	0	105	VAL
18	Р	15	GLU
18	Р	22	VAL
18	Р	26	ASP
18	Р	27	ALA
18	Р	29	PRO
18	Р	31	ALA
18	Р	44	LYS
18	Р	50	PRO
18	Р	51	VAL
18	Р	53	GLU
18	Р	68	LYS
18	Р	72	VAL
18	Р	78	LYS
19	Q	40	ASN
19	Q	67	ASP
19	Q	80	PRO
19	Q	89	ALA
19	Q	90	ARG
19	Q	96	ILE
20	R	6	ASP
20	R	11	PRO
20	R	22	ALA
20	R	30	VAL
20	R	32	PRO
20	R	48	LYS
20	R	49	VAL
$2\overline{0}$	R	60	ARG
20	R	80	ILE
$\overline{20}$	R	81	VAL
20	R	83	VAL



Mol	Chain	Res	Type
20	R	89	ILE
21	S	7	VAL
21	S	16	ALA
21	S	20	TYR
21	S	21	LYS
21	S	31	LEU
21	S	39	VAL
21	S	46	LYS
21	S	54	LYS
21	S	57	GLN
21	S	61	ILE
21	S	77	PRO
21	S	96	ILE
21	S	100	ALA
22	Т	41	LEU
22	Т	52	SER
22	Т	66	SER
22	Т	95	PRO
22	Т	146	ILE
23	U	14	ARG
23	U	17	GLN
23	U	18	ALA
23	U	45	PHE
23	U	84	LEU
24	V	11	ARG
24	V	21	ARG
24	V	51	VAL
24	V	52	ARG
24	V	80	LEU
24	V	86	SER
25	W	9	GLN
25	W	13	ALA
25	W	32	LEU
25	W	38	GLN
25	W	39	ALA
25	W	46	GLN
25	W	54	LYS
$2\overline{6}$	X	8	LEU
$2\overline{6}$	X	12	PRO
26	Х	32	GLN
$\overline{27}$	Y	29	ILE
27	Y	34	PRO



Mol	Chain	Res	Type
27	Y	37	LYS
27	Y	51	TYR
27	Y	52	TYR
28	Z	3	ARG
28	Ζ	18	PHE
28	Ζ	22	MET
28	Ζ	44	PRO
29	a	18	ALA
29	a	19	SER
29	a	26	LYS
29	a	41	ILE
30	b	6	SER
35	с	21	ARG
35	с	91	PRO
35	с	130	ARG
35	с	132	LYS
35	с	165	VAL
35	с	191	ASP
35	с	232	PRO
36	d	24	ALA
36	d	30	ARG
36	d	47	LEU
36	d	49	SER
36	d	62	ASP
36	d	111	LEU
36	d	122	GLU
36	d	127	ARG
36	d	131	ARG
36	d	151	VAL
36	d	152	ILE
36	d	161	GLU
36	d	181	ASN
37	е	5	ILE
37	е	22	LYS
37	е	29	PRO
37	е	32	ALA
37	е	67	ILE
37	е	156	GLU
37	е	172	PRO
37	е	197	PRO
37	е	207	TYR
37	e	208	SER

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Mol	Chain	Res	Type
38	f	44	GLY
38	f	70	PRO
38	f	78	HIS
38	f	101	ILE
38	f	104	ALA
38	f	128	PRO
39	g	35	ALA
39	g	100	ASN
40	h	12	LEU
40	h	20	ASP
40	h	31	MET
40	h	32	ARG
40	h	69	VAL
40	h	133	GLY
40	h	134	ALA
40	h	149	ARG
41	i	27	PRO
41	i	46	LYS
41	i	60	ARG
41	i	76	PRO
41	i	79	VAL
41	i	97	VAL
42	j	37	PHE
42	j	47	LEU
42	j	88	TYR
42	j	110	GLU
42	j	112	LYS
42	j	117	HIS
43	k	59	SER
43	k	60	ARG
43	k	99	LYS
44	1	15	ALA
44	1	50	TYR
44	1	57	THR
45	m	74	HIS
45	m	78	GLU
45	m	97	TYR
45	m	104	TYR
45	m	109	VAL
46	n	17	VAL
46	n	18	ALA
46	n	20	THR



Mol	Chain	Res	Type
46	n	100	GLY
46	n	116	THR
47	0	3	ARG
47	0	17	LYS
47	0	35	ARG
48	р	28	GLN
48	р	47	LYS
48	р	50	HIS
49	q	3	LYS
49	q	24	ALA
49	q	41	PRO
49	q	47	ASP
50	r	12	SER
50	r	45	HIS
50	r	47	PRO
50	r	68	ARG
50	r	70	ARG
50	r	94	ASN
51	s	15	ARG
51	S	33	ASP
51	s	37	VAL
51	S	59	SER
51	s	83	GLU
52	t	37	ARG
52	t	38	SER
52	t	42	PRO
52	t	65	ASN
52	t	70	LYS
52	t	78	ARG
53	u	10	LEU
53	u	42	GLN
53	u	48	LYS
53	u	71	THR
53	u	73	HIS
53	u	93	GLU
54	V	22	ARG
54	V	23	PRO
3	А	163	GLU
3	А	175	PRO
3	А	223	VAL
4	В	19	ALA
4	В	25	THR



Mol	Chain	Res	Type
4	В	84	TYR
4	В	113	VAL
4	В	114	GLY
4	В	118	VAL
4	В	174	ILE
4	В	198	ASN
4	В	204	ILE
4	В	223	GLY
4	В	232	PRO
4	В	242	ARG
4	В	272	ALA
5	С	10	GLY
5	С	12	THR
5	С	27	LEU
5	С	46	ALA
5	С	49	LEU
5	С	53	PRO
5	С	64	LYS
5	С	103	ASP
5	С	126	PRO
5	С	151	TYR
5	С	169	ASN
5	С	173	VAL
5	С	177	PRO
5	С	187	ALA
5	С	190	GLY
5	С	195	LEU
5	С	201	THR
6	D	13	ARG
6	D	16	ALA
6	D	56	GLY
6	D	65	THR
6	D	69	ARG
6	D	73	ILE
6	D	82	GLY
6	D	92	TYR
6	D	118	LEU
6	D	129	GLY
6	D	145	GLY
6	D	167	TRP
6	D	173	PRO
6	D	186	ARG



Mol	Chain	Res	Type
6	D	191	LEU
7	Е	8	LYS
7	Е	20	ILE
7	Е	28	VAL
7	Е	46	ALA
7	Е	126	ASP
8	F	9	ILE
8	F	13	LYS
8	F	17	VAL
8	F	19	VAL
8	F	21	PRO
8	F	48	GLY
8	F	119	GLU
8	F	136	ILE
8	F	168	PRO
9	G	20	ASP
9	G	23	PRO
9	G	40	THR
9	G	70	GLU
9	G	88	ILE
9	G	89	TYR
9	G	135	GLU
9	G	137	PRO
10	Н	30	LYS
10	Н	64	ASP
10	Н	84	ARG
10	Н	85	VAL
10	Н	111	GLU
10	Н	131	PRO
10	H	148	GLY
10	Н	154	GLN
10	Н	156	GLN
10	Н	158	PRO
11	Ι	26	LYS
11	Ι	28	SER
11	Ι	77	ILE
11	Ι	89	ASN
11	Ι	112	MET
11	Ι	114	ILE
12	J	13	ASN
12	J	21	ARG
12	J	47	ASP



Mol	Chain	Res	Type
12	J	83	VAL
12	J	89	ALA
12	J	94	GLU
12	J	97	PRO
12	J	115	LEU
12	J	118	GLY
13	K	6	ARG
13	K	20	ALA
13	K	28	ALA
13	K	76	LYS
13	K	119	ARG
14	L	10	LEU
14	L	28	LEU
14	L	74	LYS
15	М	20	ARG
15	М	21	THR
15	М	31	SER
15	М	46	VAL
15	М	91	PRO
15	М	92	TYR
15	М	94	TYR
15	М	96	GLY
15	М	105	ALA
16	N	22	PHE
16	N	29	ARG
16	N	47	GLY
16	N	52	ILE
16	N	68	TYR
16	N	77	PRO
16	Ν	103	ARG
16	N	116	ALA
17	0	96	ALA
17	0	103	PRO
18	Р	2	PHE
18	Р	16	PRO
18	Р	19	LYS
18	Р	36	PRO
18	Р	45	THR
18	Р	47	VAL
18	Р	74	LYS
18	Р	86	GLY
18	Р	96	ILE



Mol	Chain	Res	Type
18	Р	99	ILE
19	Q	3	ALA
19	Q	6	ILE
19	Q	7	ALA
19	Q	20	VAL
19	Q	41	LYS
19	Q	43	GLY
19	Q	63	ASP
19	Q	92	ARG
20	R	18	TYR
20	R	25	LYS
20	R	69	TYR
20	R	72	LYS
20	R	77	LYS
20	R	93	GLU
21	S	38	ILE
21	S	66	PRO
21	S	68	HIS
21	S	88	LYS
21	S	89	PHE
21	S	91	GLU
21	S	95	LYS
22	Т	50	GLN
22	Т	51	ALA
22	Т	120	ILE
22	Т	124	ILE
22	Т	152	ALA
22	Т	165	VAL
22	Т	167	PRO
23	U	13	GLY
23	U	43	THR
23	U	55	ARG
23	U	58	THR
23	U	62	LEU
23	U	63	VAL
23	U	83	PRO
24	V	14	VAL
24	V	18	ILE
24	V	56	GLN
24	V	74	VAL
$\overline{25}$	W	42	GLY
25	W	47	ASN



Mol	Chain	Res	Type
25	W	51	ARG
26	Х	50	VAL
27	Y	14	ALA
27	Y	24	ALA
29	a	35	GLN
29	a	39	LYS
29	a	51	ALA
29	a	63	PRO
35	с	9	GLU
35	с	13	ALA
35	с	32	ILE
35	с	74	LYS
35	с	95	GLN
35	с	97	TRP
35	с	131	PRO
35	с	160	ASP
35	с	181	PHE
35	с	229	VAL
36	d	12	LEU
36	d	15	THR
36	d	20	SER
36	d	29	TYR
36	d	45	LYS
36	d	50	ALA
36	d	60	ALA
36	d	63	ASN
36	d	100	ALA
36	d	108	ASN
36	d	109	PRO
36	d	156	ARG
36	d	191	THR
37	е	20	TYR
37	е	39	PRO
37	е	87	GLY
37	е	112	VAL
37	е	190	ASP
38	f	39	GLY
38	f	49	PRO
40	h	8	GLU
40	h	10	ARG
40	h	14	PRO
40	h	16	LEU



Mol	Chain	Res	Type
40	h	115	ARG
41	i	102	ARG
41	i	131	GLY
42	j	32	ASP
42	j	42	ARG
42	j	68	GLY
43	k	50	ILE
43	k	53	PRO
43	k	58	ASP
43	k	72	VAL
43	k	77	PRO
43	k	93	GLY
44	1	49	GLY
44	1	101	SER
44	1	109	VAL
45	m	7	ASN
45	m	28	GLY
45	m	30	PRO
45	m	62	GLY
45	m	71	GLY
45	m	93	PRO
45	m	106	ALA
45	m	116	ARG
45	m	118	LYS
45	m	124	PRO
46	n	6	GLY
46	n	55	ARG
46	n	64	TRP
46	n	83	ASP
46	n	101	GLN
46	n	106	ASN
47	0	21	TYR
47	0	22	THR
47	0	32	SER
47	0	34	TYR
48	р	27	VAL
48	р	49	ASP
49	q	10	GLY
49	q	12	LYS
49	q	15	PRO
49	q	31	LYS
49	q	36	ILE



Mol	Chain	Res	Type
49	q	52	ASP
50	r	10	VAL
50	r	17	LYS
50	r	31	LEU
50	r	32	TYR
50	r	33	GLY
50	r	48	GLU
50	r	62	SER
50	r	67	LYS
50	r	75	ARG
51	s	10	LYS
51	s	36	ASN
51	s	47	THR
52	t	7	LYS
52	t	52	TYR
52	t	61	TYR
53	u	41	VAL
53	u	45	GLN
53	u	47	GLY
53	u	74	LYS
53	u	98	PRO
53	u	99	LEU
54	V	15	ARG
54	V	17	THR
3	А	18	ASN
3	А	36	ALA
3	А	206	LYS
3	А	221	PRO
4	В	54	ARG
4	В	75	ILE
4	В	81	ALA
4	В	129	ASN
4	В	139	GLY
4	B	148	GLU
4	В	178	PRO
4	В	201	HIS
4	В	234	GLY
4	В	241	PRO
4	B	260	ARG
5	C	13	ARG
5	C	68	ALA
5	С	76	ARG



Mol	Chain	Res	Type
5	С	86	PRO
5	С	98	PRO
5	С	152	LYS
5	С	156	MET
6	D	5	PRO
6	D	8	SER
6	D	10	SER
6	D	26	HIS
6	D	40	ARG
6	D	41	ARG
6	D	61	PRO
6	D	90	ARG
6	D	108	ALA
6	D	148	SER
7	Е	73	ALA
7	Е	117	PHE
7	Е	147	ASP
8	F	47	GLU
8	F	59	ARG
8	F	102	ALA
8	F	118	PRO
8	F	135	GLY
8	F	158	HIS
8	F	165	ALA
9	G	7	GLU
9	G	25	TYR
9	G	81	VAL
9	G	86	THR
9	G	91	SER
9	G	95	LYS
9	G	126	TYR
10	Н	31	GLN
11	Ι	30	ALA
11	Ι	61	VAL
11	Ι	64	ARG
12	J	72	PRO
12	J	145	PRO
13	K	84	GLY
13	K	91	GLU
13	K	115	MET
14	L	6	SER
14	L	50	HIS



Mol	Chain	Res	Type
14	L	67	LEU
14	L	94	TYR
14	L	108	GLY
15	М	25	ARG
15	М	28	VAL
15	М	29	PHE
15	М	47	THR
15	М	64	GLU
16	Ν	2	ASN
16	Ν	5	ALA
16	Ν	36	GLU
16	Ν	93	ARG
16	Ν	112	ARG
17	0	23	GLY
17	0	24	TYR
17	0	93	LYS
17	0	102	GLU
17	0	116	ALA
18	Р	20	LEU
18	Р	24	LYS
18	Р	59	ALA
18	Р	79	VAL
19	Q	42	ARG
19	Q	73	ALA
19	Q	88	ARG
20	R	34	ALA
20	R	59	VAL
20	R	65	ARG
20	R	78	LYS
21	S	9	LYS
21	S	10	GLY
21	S	25	GLY
21	S	29	GLU
21	S	33	LYS
21	S	60	PHE
21	S	65	ALA
21	S	67	LEU
21	S	78	ALA
21	S	101	LYS
22	Т	83	PRO
22	Т	90	VAL
22	Т	122	ARG



Mol	Chain	Res	Type
23	U	19	LYS
23	U	25	ARG
23	U	70	GLN
24	V	32	LYS
24	V	63	ALA
25	W	14	ARG
25	W	60	LEU
26	Х	31	LEU
29	a	31	HIS
29	a	42	ARG
30	b	12	ASP
35	С	54	THR
35	с	60	ASP
35	с	100	GLY
35	С	149	LEU
36	d	43	LEU
36	d	123	GLN
36	d	163	ALA
36	d	178	LEU
37	е	44	GLY
37	е	49	ARG
37	е	147	ALA
38	f	71	LEU
38	f	117	ASP
39	g	81	ILE
39	g	93	SER
40	h	41	ARG
40	h	63	LYS
40	h	73	MET
40	h	90	GLU
40	h	117	ALA
40	h	129	GLU
41	i	20	TYR
41	i	74	PRO
41	i	91	ARG
41	i	107	LEU
41	i	121	ASP
42	j	29	ASN
43	k	12	ASP
43	k	15	THR
44	1	44	SER
44	l	89	ALA



Mol	Chain	Res	Type
45	m	44	PRO
45	m	103	VAL
46	n	27	LYS
46	n	46	LYS
46	n	67	GLU
47	0	5	ALA
47	0	14	PRO
47	0	18	VAL
48	р	32	LEU
48	р	33	THR
48	р	55	GLY
48	р	56	LEU
48	р	72	ARG
48	р	79	ARG
49	q	13	HIS
49	q	26	ARG
49	q	29	ASP
49	q	30	GLY
49	q	34	GLU
49	q	65	GLN
50	r	83	ASP
51	s	25	THR
51	s	53	ARG
51	S	76	LEU
51	s	82	THR
52	t	5	LEU
52	t	6	LYS
52	t	9	VAL
52	t	28	LYS
52	t	35	SER
$5\overline{2}$	t	46	GLY
$5\overline{4}$	v	3	LYS
3	A	19	LYS
3	A	23	ILE
3	A	203	GLU
3	A	207	GLY
4	В	5	LYS
4	В	9	TYR
4	В	35	LYS
4	В	123	ALA
4	В	124	PRO
4	В	159	ALA



Mol	Chain	Res	Type
4	В	224	ALA
5	С	45	THR
5	С	125	GLY
5	С	153	GLY
5	С	202	LYS
6	D	39	ARG
6	D	70	HIS
6	D	88	LYS
6	D	103	LYS
6	D	179	TYR
6	D	185	GLU
7	Е	25	TYR
7	Е	76	SER
7	Е	122	PRO
8	F	30	LYS
8	F	81	GLU
8	F	126	PRO
8	F	152	ARG
9	G	62	LYS
9	G	74	ASN
10	Н	33	GLU
10	Н	40	ASP
10	Н	42	GLU
10	Н	141	LYS
11	Ι	31	LYS
11	Ι	49	ARG
11	Ι	50	GLY
11	Ι	120	GLU
12	J	23	PRO
12	J	48	PRO
12	J	79	ARG
12	J	108	LYS
12	J	146	VAL
13	K	8	LYS
13	K	23	GLY
13	K	32	PHE
13	K	40	ALA
13	K	125	LEU
13	K	135	ASP
14	L	8	ARG
14	L	46	GLY
15	М	23	ARG



Mol	Chain	Res	Type
16	N	24	PRO
16	N	32	TYR
16	N	41	ARG
16	N	55	ASN
16	N	131	ALA
16	N	133	GLU
17	0	53	ARG
17	0	77	SER
17	0	91	ASP
19	Q	46	PHE
20	R	7	VAL
20	R	90	GLU
21	S	12	THR
21	S	15	VAL
21	S	18	GLY
21	S	40	GLU
22	Т	2	GLU
22	Т	39	VAL
22	Т	153	SER
23	U	27	GLU
23	U	41	ARG
24	V	62	VAL
24	V	88	LYS
25	W	15	LYS
26	Х	9	VAL
35	с	56	ARG
35	с	182	ILE
35	с	209	ARG
35	с	237	ALA
36	d	17	ASP
36	d	129	ALA
36	d	168	ALA
36	d	175	LEU
37	е	101	LEU
38	f	73	ASN
40	h	33	ASP
40	h	36	LYS
40	h	53	LYS
40	h	70	LYS
41	i	52	ASP
42	j	7	THR
42	j	10	ARG



Mol	Chain	Res	Type
42	j	97	LYS
43	k	71	LEU
44	l	54	ARG
45	m	29	ALA
46	n	105	THR
46	n	117	VAL
47	0	33	VAL
49	q	23	ASP
49	q	28	ARG
49	q	42	ARG
49	q	70	ALA
50	r	50	LYS
50	r	77	VAL
51	s	9	LYS
52	t	20	LEU
52	t	55	LYS
52	t	67	VAL
53	u	43	LEU
54	V	20	LYS
4	В	45	ASN
4	В	47	GLY
4	В	53	PHE
4	В	87	ASN
4	В	116	GLN
4	В	268	ARG
5	С	180	ASN
6	D	12	ARG
6	D	50	GLY
6	D	52	VAL
6	D	83	VAL
6	D	97	PRO
6	D	163	ARG
7	Е	107	LEU
7	Е	146	TYR
8	F	15	VAL
8	F	38	SER
8	F	170	ARG
10	Н	119	GLU
10	Н	130	LEU
11	Ι	24	VAL
11	Ι	94	ARG
11	Ι	103	ALA



Mol	Chain	Res	Type
12	J	61	ARG
12	J	78	PRO
12	J	129	ALA
13	K	2	LEU
13	K	49	ALA
13	K	63	LYS
13	K	121	ALA
13	K	132	VAL
15	М	48	LEU
15	М	56	LEU
16	N	95	ARG
16	N	128	GLU
18	Р	23	GLU
18	Р	58	VAL
18	Р	84	LYS
18	Р	90	PRO
19	Q	98	LYS
21	S	3	VAL
21	S	34	LYS
21	S	56	PRO
21	S	86	ARG
22	Т	16	SER
22	Т	53	ILE
22	Т	168	GLU
23	U	20	ARG
23	U	23	VAL
23	U	33	ALA
24	V	68	PRO
25	W	11	GLU
25	W	16	LEU
26	Х	18	ASP
29	a	59	LYS
30	b	14	CYS
35	с	19	HIS
35	с	98	LEU
35	с	178	ARG
36	d	9	GLY
36	d	115	LEU
36	d	172	ARG
36	d	204	LEU
37	е	9	CYS
37	е	132	ARG



Mol	Chain	Res	Type
38	f	143	ARG
39	g	48	LEU
39	g	78	GLU
39	g	88	VAL
40	h	9	VAL
40	h	88	PRO
41	i	24	THR
42	j	54	ASP
43	k	76	ASN
43	k	98	ILE
44	1	39	PRO
45	m	70	PRO
46	n	99	ARG
46	n	119	GLY
49	q	66	PRO
50	r	95	TYR
52	t	8	GLY
54	V	18	TYR
54	V	19	GLY
4	В	251	GLY
5	С	30	PRO
5	С	188	VAL
6	D	89	PRO
8	F	11	VAL
8	F	42	ARG
8	F	82	GLY
8	F	151	ILE
10	Н	109	PRO
11	Ι	22	ILE
11	Ι	76	ALA
11	Ι	113	LYS
12	J	8	PRO
13	K	111	GLU
14	L	38	VAL
16	N	20	PRO
$1\overline{6}$	N	90	GLN
17	0	20	LEU
17	0	88	ILE
19	Q	35	ILE
20	R	88	LYS
$\overline{21}$	S	30	VAL
21	S	52	SER



Mol	Chain	Res	Type
22	Т	12	GLY
23	U	57	PHE
25	W	57	ILE
$\frac{20}{27}$	V	55	ARG
29	a	4	MET
29	a	38	GLY
30	h	10	ILE
30	h	30	PRO
35	C	23	ARG
35	C C	120	ILE
36	d	61	ALA
36	d	81	GLY
36	d	174	PRO
37	e u	51	PRO
40	b b	81	GLV
<u> </u>	i	13/	ILE
41	i	53	VAL
42	J	80	SEB
40 50	- 111 - r	16	
50	r	64	BBO
52	1 +	76	PRO
3		204	CLV
<u> </u>	B	74	GLI
4	B	195	UE
4	D	80	CLV
16	D N	10	IFU
10	D N	19 65	
27	I V	41	PRO
21	1	41	PPO
20	L h	1 25	VAL
30	d	 	VAL
30 27	u o	00	CLV
२१ २०	e f	90 100	
<u>ა</u> ბ 1	1	100	VAL IIE
41	1 1-	0 74	
43 50	К +	14	
02 E		49	
0 7		139	
( 0		119	GLY
8 10		51	GLY
10	H		VAL
10	H	157	AKG
11		72	PRO



Mol	Chain	Res	Type
21	S	45	VAL
21	S	80	GLY
27	Y	33	CYS
38	f	93	PRO
40	h	91	VAL
47	0	56	VAL
49	q	19	ILE
4	В	229	VAL
4	В	246	PRO
5	С	184	VAL
6	D	121	VAL
8	F	121	ILE
9	G	124	GLY
11	Ι	19	ILE
11	Ι	101	PRO
12	J	20	GLY
16	N	88	ILE
17	0	82	GLY
22	Т	42	VAL
24	V	12	PRO
37	е	37	PRO
37	е	136	PRO
44	1	48	ILE
50	r	46	ASP
52	t	54	GLY
53	u	100	ILE
4	В	92	ILE
4	В	106	ILE
4	В	216	GLY
4	В	244	ARG
5	С	47	VAL
5	С	141	ILE
10	Н	149	PRO
11	Ι	86	ILE
12	J	19	VAL
15	М	85	VAL
16	Ν	66	VAL
30	b	3	VAL
35	с	164	VAL
37	e	133	VAL
41	i	26	VAL
43	k	41	PRO



Mol	Chain	Res	Type
50	r	5	VAL
50	r	19	VAL
53	u	97	ALA
3	А	52	PRO
5	С	116	VAL
12	J	62	LEU
23	U	79	VAL
27	Y	6	VAL
39	g	72	VAL
41	i	4	ASP
44	1	21	ILE
4	В	245	PRO

## 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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
3	А	106/181~(59%)	86 (81%)	20 (19%)	1 10
4	В	214/218~(98%)	179 (84%)	35~(16%)	2 15
5	С	163/166~(98%)	130 (80%)	33 (20%)	1 9
6	D	154/162~(95%)	133~(86%)	21 (14%)	3 21
7	Е	154/156~(99%)	130 (84%)	24 (16%)	2 17
8	F	142/148~(96%)	129 (91%)	13~(9%)	9 35
9	G	124/124~(100%)	100 (81%)	24 (19%)	1 9
10	Н	117/119~(98%)	96~(82%)	21 (18%)	2 12
11	Ι	100/100~(100%)	74 (74%)	26 (26%)	0 4
12	J	112/116~(97%)	91 (81%)	21 (19%)	1 10
13	Κ	108/111~(97%)	84 (78%)	24 (22%)	1 7
14	L	101/101 (100%)	89 (88%)	12 (12%)	5 25
15	М	84/88~(96%)	71 (84%)	13 (16%)	2 17
16	Ν	121/128 (94%)	101 (84%)	20 (16%)	2 15



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Mol	Chain	Analysed	Rotameric	Outliers	Pere	centil	$\mathbf{es}$
17	Ο	93/94~(99%)	77 (83%)	16 (17%)	2	13	
18	Р	82/82~(100%)	64 (78%)	18 (22%)	1	7	
19	Q	89/92~(97%)	75 (84%)	14 (16%)	2	17	
20	R	74/78~(95%)	62 (84%)	12 (16%)	2	15	
21	S	86/91~(94%)	73 (85%)	13 (15%)	3	18	
22	Т	163/179~(91%)	136 (83%)	27 (17%)	2	14	
23	U	61/67~(91%)	54 (88%)	7 (12%)	5	27	
24	V	73/83~(88%)	61 (84%)	12 (16%)	2	15	
25	W	58/67~(87%)	47 (81%)	11 (19%)	1	10	
26	Х	52/52~(100%)	46 (88%)	6 (12%)	5	27	
27	Y	49/52~(94%)	40 (82%)	9 (18%)	1	11	
28	Ζ	41/42~(98%)	34 (83%)	7 (17%)	2	14	
29	a	53/55~(96%)	44 (83%)	9 (17%)	2	14	
30	b	33/34~(97%)	31 (94%)	2 (6%)	18	50	
35	с	202/220~(92%)	169 (84%)	33 (16%)	2	15	
36	d	160/188~(85%)	130 (81%)	30 (19%)	1	10	
37	е	180/181 (99%)	154 (86%)	26 (14%)	3	19	
38	f	115/123 (94%)	102 (89%)	13 (11%)	6	27	
39	g	90/90~(100%)	77 (86%)	13 (14%)	3	19	
40	h	126/127~(99%)	108 (86%)	18 (14%)	3	20	
41	i	119/119~(100%)	96 (81%)	23 (19%)	1	10	
42	j	98/99~(99%)	89 (91%)	9 (9%)	9	35	
43	k	88/92~(96%)	76 (86%)	12 (14%)	3	21	
44	1	88/99~(89%)	78 (89%)	10 (11%)	5	27	
45	m	104/109~(95%)	80 (77%)	24 (23%)	1	6	
46	n	100/101 (99%)	75 (75%)	25 (25%)	0	4	
47	О	49/50~(98%)	37 (76%)	12 (24%)	0	5	
48	р	79/80~(99%)	66 (84%)	13 (16%)	2	15	
49	q	72/74~(97%)	57 (79%)	15 (21%)	1	8	
50	r	96/97~(99%)	79 (82%)	17 (18%)	2	12	
51	s	71/77~(92%)	63 (89%)	8 (11%)	6	27	



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
52	t	71/80~(89%)	52~(73%)	19 (27%)	0 3
53	u	76/82~(93%)	66 (87%)	10 (13%)	4 22
54	V	19/22~(86%)	16 (84%)	3~(16%)	2 16
All	All	4810/5096~(94%)	4007 (83%)	803 (17%)	2 14

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All (803) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	А	8	TYR
3	А	12	LEU
3	А	16	ASP
3	А	19	LYS
3	А	20	ILE
3	А	21	TYR
3	А	22	THR
3	А	30	VAL
3	А	32	GLU
3	А	43	GLU
3	А	53	ARG
3	А	163	GLU
3	А	165	ARG
3	А	178	LYS
3	А	189	ASN
3	А	193	PHE
3	А	197	LEU
3	А	198	GLU
3	А	201	LYS
3	А	209	PHE
4	В	10	THR
4	В	13	ARG
4	В	15	PHE
4	В	18	VAL
4	В	24	ILE
4	В	31	LYS
4	В	33	LEU
4	В	37	LEU
4	В	43	ARG
4	В	60	ARG
4	В	61	LEU
4	В	63	ARG
4	В	66	ASP



Mol	Chain	Res	Type
4	В	67	PHE
4	В	70	TRP
4	В	71	ASP
4	В	79	VAL
4	В	115	GLN
4	В	131	LEU
4	В	150	LYS
4	В	164	GLN
4	В	176	ARG
4	В	177	LEU
4	В	198	ASN
4	В	201	HIS
4	В	213	ARG
4	В	214	TRP
4	В	217	ARG
4	В	229	VAL
4	В	242	ARG
4	В	255	LYS
4	В	257	LEU
4	В	262	ARG
4	В	263	ARG
4	В	271	ILE
5	С	5	LEU
5	С	12	THR
5	С	15	PHE
5	С	19	ARG
5	С	21	VAL
5	С	23	VAL
5	С	24	THR
5	С	27	LEU
5	С	37	ARG
5	С	42	ASP
5	С	44	TYR
5	С	61	ARG
5	С	66	HIS
5	C	67	PHE
5	С	78	LEU
5	С	79	ARG
5	С	84	PHE
5	С	89	ASP
5	С	97	LYS
5	С	107	THR



Mol	Chain	Res	Type
5	С	117	MET
5	С	119	ARG
5	С	122	PHE
5	С	141	ILE
5	С	156	MET
5	С	173	VAL
5	С	179	GLU
5	С	183	LEU
5	С	188	VAL
5	С	192	ASN
5	С	197	ILE
5	С	201	THR
5	С	203	LYS
6	D	22	GLU
6	D	27	LEU
6	D	77	ILE
6	D	83	VAL
6	D	84	VAL
6	D	92	TYR
6	D	97	PRO
6	D	115	GLU
6	D	117	LYS
6	D	120	LEU
6	D	135	LEU
6	D	137	TRP
6	D	143	LEU
6	D	144	ASP
6	D	149	VAL
6	D	165	LEU
6	D	179	TYR
6	D	180	ASP
6	D	181	ILE
6	D	183	ARG
6	D	196	VAL
7	Е	10	LYS
7	Е	12	TYR
7	Е	19	LEU
7	Е	25	TYR
7	Е	29	TRP
7	Е	31	VAL
7	Е	33	ARG
7	E	55	LYS



Mol	Chain	Res	Type
7	Е	72	ARG
7	Е	80	PHE
7	Е	95	ARG
7	Е	99	MET
7	Е	115	ARG
7	Е	135	LEU
7	Е	136	ARG
7	Е	138	GLN
7	Е	139	LEU
7	Е	146	TYR
7	Е	148	MET
7	Е	155	MET
7	Е	165	THR
7	Е	173	LEU
7	Е	176	LEU
7	Е	178	PHE
8	F	65	HIS
8	F	68	THR
8	F	87	LEU
8	F	89	ILE
8	F	90	LYS
8	F	92	ILE
8	F	98	LEU
8	F	110	SER
8	F	139	GLN
8	F	140	LYS
8	F	152	ARG
8	F	162	ILE
8	F	172	LYS
9	G	3	VAL
9	G	20	ASP
9	G	21	VAL
9	G	27	ARG
9	G	31	LEU
9	G	33	ARG
9	G	38	LEU
9	G	41	GLU
9	G	44	LEU
9	G	62	LYS
9	G	76	THR
9	G	77	LEU
9	G	93	THR



Mol	Chain	Res	Type
9	G	96	ASP
9	G	99	GLU
9	G	103	ARG
9	G	108	THR
9	G	109	ILE
9	G	114	LEU
9	G	118	LYS
9	G	123	LEU
9	G	130	TYR
9	G	136	VAL
9	G	139	GLN
10	Н	25	LYS
10	Н	33	GLU
10	Н	35	ARG
10	Н	38	LEU
10	Н	60	LYS
10	Н	62	ARG
10	Н	71	MET
10	Н	84	ARG
10	Н	86	THR
10	Н	92	GLN
10	Н	95	TYR
10	Н	98	TYR
10	Н	129	MET
10	Н	132	LYS
10	Н	140	PHE
10	Н	142	ARG
10	Н	143	LEU
10	Н	145	VAL
10	Н	146	TYR
10	Н	159	GLU
10	H	161	LEU
11	Ι	1	MET
11	I	3	GLN
11	Ι	9	GLU
11	Ι	10	VAL
11	Ι	12	ASP
11	Ι	21	CYS
11	Ι	29	ASN
11	Ι	39	ILE
11	I	45	GLU
11	Ι	49	ARG



Mol	Chain	Res	Type
11	Ι	58	VAL
11	Ι	59	LYS
11	Ι	63	VAL
11	Ι	67	LYS
11	Ι	68	GLU
11	Ι	77	ILE
11	Ι	80	ASP
11	Ι	91	LEU
11	Ι	96	THR
11	Ι	97	ARG
11	Ι	102	VAL
11	Ι	104	ARG
11	Ι	105	GLU
11	Ι	109	LYS
11	Ι	114	ILE
11	Ι	120	GLU
12	J	5	ASP
12	J	13	ASN
12	J	45	LEU
12	J	60	MET
12	J	61	ARG
12	J	62	LEU
12	J	68	GLN
12	J	74	GLU
12	J	77	ARG
12	J	80	TYR
12	J	81	GLN
12	J	84	ASN
12	J	85	LEU
12	J	96	THR
12	J	100	LEU
12	J	110	TYR
12	J	121	LYS
12	J	130	PHE
12	J	145	PRO
12	J	148	LEU
12	J	149	GLU
13	Κ	3	MET
13	K	8	LYS
13	K	9	TYR
13	Κ	11	LYS
13	K	14	ARG


Mol	Chain	Res	Type
13	K	17	LEU
13	K	25	ASP
13	K	29	PHE
13	K	32	PHE
13	K	41	TRP
13	K	42	ILE
13	Κ	51	ARG
13	Κ	59	ARG
13	Κ	64	ILE
13	Κ	65	PHE
13	K	69	PHE
13	Κ	82	ARG
13	Κ	89	ASN
13	Κ	93	TYR
13	Κ	103	MET
13	Κ	111	GLU
13	Κ	124	LYS
13	Κ	133	ARG
13	Κ	134	ARG
14	L	9	LYS
14	L	14	SER
14	L	29	LEU
14	L	31	HIS
14	L	38	VAL
14	L	43	GLU
14	L	59	ASP
14	L	65	LEU
14	L	68	ARG
14	L	88	ARG
14	L	94	TYR
14	L	105	ARG
15	М	7	TYR
15	М	10	ARG
15	М	12	PHE
15	М	14	VAL
15	М	15	ARG
15	М	24	LEU
15	М	39	ILE
15	М	42	ASP
15	М	46	VAL
15	М	54	LEU
15	М	75	GLU



Mol	Chain	Res	Type
15	М	93	LYS
15	М	94	TYR
16	N	6	LEU
16	N	32	TYR
16	N	35	LYS
16	N	38	ASN
16	N	57	PHE
16	N	61	PHE
16	N	62	THR
16	N	85	LYS
16	N	87	ASP
16	N	88	ILE
16	N	98	LYS
16	N	103	ARG
16	N	107	ASP
16	N	111	ARG
16	N	112	ARG
16	N	113	LYS
16	N	118	ARG
16	N	121	ILE
16	N	123	LYS
16	N	124	ASP
17	0	5	LYS
17	0	14	HIS
17	0	25	TRP
17	0	27	LEU
17	0	51	LYS
17	0	58	ARG
17	0	71	GLN
17	0	74	LEU
17	0	79	PHE
17	0	84	LYS
17	0	85	LYS
17	0	91	ASP
17	0	97	ASP
17	0	106	PHE
17	0	109	LEU
17	0	114	LYS
18	Р	13	ARG
18	Р	18	LEU
18	Р	20	LEU
18	Р	23	GLU



Mol	Chain	Res	Type
18	Р	26	ASP
18	Р	35	LEU
18	Р	39	LEU
18	Р	40	LEU
18	Р	51	VAL
18	Р	58	VAL
18	Р	60	GLU
18	Р	62	LEU
18	Р	80	GLN
18	Р	81	TYR
18	Р	82	ARG
18	Р	89	GLN
18	Р	92	THR
18	Р	98	GLU
19	Q	6	ILE
19	Q	8	ARG
19	Q	21	VAL
19	Q	23	LEU
19	Q	31	GLU
19	Q	49	LYS
19	Q	51	LEU
19	Q	67	ASP
19	Q	68	ARG
19	Q	70	TYR
19	Q	76	VAL
19	Q	86	LEU
19	Q	88	ARG
19	Q	97	LYS
20	R	3	THR
20	R	13	LEU
20	R	26	TYR
20	R	27	THR
20	R	38	GLU
20	R	49	VAL
20	R	56	THR
$\overline{20}$	R	62	LYS
20	R	65	ARG
20	R	76	ARG
20	R	77	LYS
20	R	83	VAL
21	S	9	LYS
21	S	20	TYR



Mol	Chain	Res	Type
21	S	23	ARG
21	S	28	LYS
21	S	40	GLU
21	S	44	ILE
21	S	50	ARG
21	S	64	GLU
21	S	67	LEU
21	S	71	LYS
21	S	73	ARG
21	S	75	ILE
21	S	97	ARG
22	Т	1	MET
22	Т	8	TYR
22	Т	9	TYR
22	Т	19	ARG
22	Т	20	ARG
22	Т	31	ARG
22	Т	41	LEU
22	Т	44	PHE
22	Т	48	PHE
22	Т	50	GLN
22	Т	53	ILE
22	Т	78	LYS
22	Т	80	ARG
22	Т	88	PHE
22	Т	95	PRO
22	Т	104	PHE
22	Т	119	GLU
22	Т	144	LEU
22	Т	145	GLU
22	Т	146	ILE
22	Т	150	LEU
22	Т	151	HIS
22	Т	157	LEU
22	Т	162	GLU
22	Т	163	LEU
22	Т	170	THR
22	Т	171	ILE
23	U	19	LYS
23	U	20	ARG
23	U	$\overline{26}$	TYR
23	U	53	MET



Mol	Chain	Res	Type
23	U	62	LEU
23	U	64	ASP
23	U	69	PHE
24	V	13	ILE
24	V	18	ILE
24	V	26	ARG
24	V	41	ARG
24	V	43	TYR
24	V	46	LEU
24	V	58	ILE
24	V	60	PHE
24	V	62	VAL
24	V	78	LYS
24	V	85	LEU
24	V	91	LYS
25	W	9	GLN
25	W	12	GLU
25	W	14	ARG
25	W	15	LYS
25	W	27	GLU
25	W	29	LYS
25	W	33	MET
25	W	37	PHE
25	W	47	ASN
25	W	48	HIS
25	W	55	ARG
26	Х	8	LEU
26	Х	23	LEU
26	Х	29	ARG
26	Х	30	ARG
26	Х	35	ARG
26	Х	49	LYS
27	Y	16	ARG
27	Y	25	LEU
27	Y	26	THR
27	Y	29	ILE
27	Y	33	CYS
27	Y	39	MET
27	Y	49	CYS
27	Y	51	TYR
27	Y	56	LYS
28	Ζ	1	MET



Mol	Chain	Res	Type
28	Z	2	LYS
$\frac{-3}{28}$	Z	5	TRP
28	Z	15	THR
28	<u>Z</u>	29	LYS
$\frac{20}{28}$	Z	39	ARG
28	Z	44	PRO
29	a	3	LYS
29	a	16	ILE
29	a	17	THR
29	a	25	MET
29	a	34	TRP
29	a	36	LYS
29	a	44	LYS
29	a	48	PHE
29	a	60	LEU
30	b	24	TYR
30	b	25	VAL
35	c	8	LYS
35	c	10	LEU
35	c	17	PHE
35	c	19	HIS
35	c	23	ARG
35	с	42	ILE
35	c	47	THR
35	с	48	MET
35	с	51	LEU
35	С	60	ASP
35	с	67	THR
35	с	71	VAL
35	с	92	TYR
35	с	101	MET
35	с	102	LEU
35	с	118	LEU
35	с	132	LYS
35	с	133	LYS
35	с	136	VAL
35	с	137	ARG
35	с	143	GLU
35	с	146	GLN
35	с	149	LEU
35	с	155	LEU
35	с	156	LYS



Mol	Chain	Res	Type
35	с	164	VAL
35	с	169	LYS
35	с	172	ILE
35	с	200	ILE
35	с	204	ASN
35	с	209	ARG
35	с	220	ASP
35	с	221	LEU
36	d	3	ASN
36	d	4	LYS
36	d	16	ARG
36	d	27	LYS
36	d	29	TYR
36	d	32	LEU
36	d	33	LEU
36	d	46	GLU
36	d	52	LEU
36	d	56	ASP
36	d	84	ILE
36	d	93	LYS
36	d	94	LEU
36	d	95	THR
36	d	97	LYS
36	d	102	ASN
36	d	107	GLN
36	d	111	LEU
36	d	118	GLN
36	d	123	GLN
36	d	126	ARG
36	d	130	VAL
36	d	131	ARG
36	d	135	LYS
36	d	139	GLN
36	d	175	LEU
36	d	178	LEU
36	d	186	PHE
36	d	193	TYR
36	d	195	VAL
37	е	8	VAL
37	e	14	ARG
37	е	15	GLU
37	е	22	LYS



37e $29$ PRO $37$ e $33$ MET $37$ e $36$ ARG $37$ e $39$ PRO $37$ e $59$ ARG $37$ e $61$ LYS $37$ e $68$ TYR $37$ e $72$ GLU $37$ e $72$ GLU $37$ e $78$ LEU $37$ e $79$ PHE $37$ e $94$ LEU $37$ e $97$ LEU $37$ e $101$ LEU $37$ e $104$ VAL $37$ e $120$ LEU $37$ e $134$ ASP $37$ e $134$ ASP $37$ e $199$ ASN $37$ e $203$ VAL $37$ e $203$ VAL $37$ e $203$ VAL $37$ e $203$ VAL $37$ e $199$ ASN $37$ e $203$ VAL $37$ e $203$ VAL $37$ e $203$ VAL $37$ e $203$ VAL $37$ $38$ f $6$ $99$ $38$ f $10$ $38$ f $10$ $38$ $38$ f $12$ $128$ $38$ f $57$ $128$ $38$ f $57$ $128$ $38$ f $72$ $GLN$	Mol	Chain	Res	Type
37e $33$ MET $37$ e $36$ ARG $37$ e $39$ PRO $37$ e $59$ ARG $37$ e $61$ LYS $37$ e $68$ TYR $37$ e $72$ GLU $37$ e $72$ GLU $37$ e $78$ LEU $37$ e $79$ PHE $37$ e $94$ LEU $37$ e $97$ LEU $37$ e $101$ LEU $37$ e $104$ VAL $37$ e $120$ LEU $37$ e $134$ ASP $37$ e $188$ LEU $37$ e $191$ ARG $37$ e $203$ VAL $37$ e $203$ VAL $37$ e $207$ TYR $38$ f $6$ PHE $38$ f $10$ MET $38$ f $12$ LEU $38$ f $72$	37	е	29	PRO
37e $36$ ARG $37$ e $39$ PRO $37$ e $59$ ARG $37$ e $61$ LYS $37$ e $68$ TYR $37$ e $72$ GLU $37$ e $72$ GLU $37$ e $79$ PHE $37$ e $94$ LEU $37$ e $97$ LEU $37$ e $101$ LEU $37$ e $104$ VAL $37$ e $120$ LEU $37$ e $120$ LEU $37$ e $134$ ASP $37$ e $134$ ASP $37$ e $191$ ARG $37$ e $203$ VAL $37$ e $203$ VAL $37$ e $203$ VAL $37$ e $100$ MET $38$ f $6$ PHE $38$ f $10$ MET $38$ f $12$ LEU $38$ f $72$ GLN	37	е	33	MET
37e $39$ PRO $37$ e $59$ ARG $37$ e $61$ LYS $37$ e $68$ TYR $37$ e $72$ GLU $37$ e $78$ LEU $37$ e $79$ PHE $37$ e $94$ LEU $37$ e $97$ LEU $37$ e $101$ LEU $37$ e $104$ VAL $37$ e $120$ LEU $37$ e $120$ LEU $37$ e $122$ ARG $37$ e $134$ ASP $37$ e $191$ ARG $37$ e $203$ VAL $37$ e $203$ VAL $37$ e $203$ VAL $37$ e $203$ VAL $37$ e $207$ TYR $38$ f $6$ PHE $38$ f $10$ MET $38$ f $12$ LEU $38$ f $43$ LEU $38$ f $43$ LEU $38$ f $43$ LEU $38$ f $72$ GLN	37	е	36	ARG
37e $59$ ARG $37$ e $61$ LYS $37$ e $68$ TYR $37$ e $72$ GLU $37$ e $72$ GLU $37$ e $79$ PHE $37$ e $94$ LEU $37$ e $97$ LEU $37$ e $97$ LEU $37$ e $101$ LEU $37$ e $104$ VAL $37$ e $120$ LEU $37$ e $122$ ARG $37$ e $134$ ASP $37$ e $191$ ARG $37$ e $191$ ARG $37$ e $203$ VAL $37$ e $203$ VAL $37$ e $207$ TYR $38$ f $6$ PHE $38$ f $10$ MET $38$ f $12$ LEU $38$ f $43$ LEU $38$ f $57$ LYS $38$ f $72$ GLN	37	е	39	PRO
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	37	е	59	ARG
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	37	е	61	LYS
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	37	е	68	TYR
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	37	е	72	GLU
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	37	е	78	LEU
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	37	е	79	PHE
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	37	е	94	LEU
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	37	е	97	LEU
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	37	е	101	LEU
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	37	е	104	VAL
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	37	е	120	LEU
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	37	е	122	ARG
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	37	е	134	ASP
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	37	е	188	LEU
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	37	е	191	ARG
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	37	е	199	ASN
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	37	е	203	VAL
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	37	е	207	TYR
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	38	f	6	PHE
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	38	f	10	MET
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	38	f	12	LEU
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	38	f	43	LEU
38 f 72 GLN	38	f	57	LYS
	38	f	72	GLN
38 f 78 HIS	38	f	78	HIS
38 f 105 VAL	38	f	105	VAL
38 f 118 ILE	38	f	118	ILE
38 f 136 MET	38	f	136	MET
38 <u>f</u> 137 GLU	38	f	137	GLU
38 f 143 ARG	38	f	143	ARG
38 f 144 THR	38	f	144	THR
39 g 2 ARG	39	g	2	ARG
39 g 15 ASP	39	g	15	ASP
39 g 17 SER	39	g	17	SER
39 g 27 GLN	39	g	27	GLN
39 g 37 VAL	39	g	37	VAL
39 g 43 LEU	39	g	43	LEU
39 g 55 ASP	39	g	55	ASP



39         g         75         LEU           39         g         78         GLU           39         g         83         ASP           39         g         86         ARG           39         g         91         VAL           39         g         100         ASN           40         h         4         ARG           40         h         29         LYS           40         h         32         ARG           40         h         32         ARG           40         h         32         ARG           40         h         35         LYS           40         h         35         LYS           40         h         43         PHE           40         h         43         PHE           40         h         64         GLN           40         h         64         ASN           40         h         103         TRP           40         h         103         TRP           40         h         155         ARG           41         i         1	Mol	Chain	Res	Tvpe
39         g         78         GLU           39         g         83         ASP           39         g         86         ARG           39         g         91         VAL           39         g         91         VAL           39         g         91         VAL           39         g         91         VAL           39         g         100         ASN           40         h         4         ARG           40         h         29         LYS           40         h         32         ARG           40         h         35         LYS           40         h         35         LYS           40         h         43         PHE           40         h         43         PHE           40         h         64         GLN           40         h         68         ASN           40         h         103         TRP           40         h         103         TRP           40         h         155         ARG           41         i         1	39	g	75	LEU
39         g         83         ASP           39         g         83         ASP           39         g         91         VAL           39         g         91         VAL           39         g         100         ASN           40         h         4         ARG           40         h         29         LYS           40         h         29         LYS           40         h         32         ARG           40         h         32         ARG           40         h         35         LYS           40         h         43         PHE           40         h         43         PHE           40         h         43         PHE           40         h         64         GLN           40         h         103         TRP           40         h         103         TRP           40         h         113         GLU           40         h         155         ARG           41         i         1         MET           41         i         2	39	g	78	GLU
39         g         86         ARG           39         g         91         VAL           39         g         100         ASN           40         h         4         ARG           40         h         5         ARG           40         h         29         LYS           40         h         32         ARG           40         h         32         ARG           40         h         35         LYS           40         h         35         LYS           40         h         43         PHE           40         h         43         PHE           40         h         59         LEU           40         h         64         GLN           40         h         103         TRP           40         h         103         TRP           40         h         113         GLU           40         h         155         ARG           40         h         155         ARG           41         i         1         MET           41         i         1	39	g	83	ASP
39         g         91         VAL           39         g         100         ASN           40         h         4         ARG           40         h         5         ARG           40         h         29         LYS           40         h         32         ARG           40         h         32         ARG           40         h         32         ARG           40         h         35         LYS           40         h         35         LYS           40         h         43         PHE           40         h         59         LEU           40         h         64         GLN           40         h         68         ASN           40         h         103         TRP           40         h         103         TRP           40         h         151         TYR           40         h         155         ARG           41         i         1         MET           41         i         17         THR           41         i         17	39	g	86	ARG
39         g         100         ASN           40         h         4         ARG           40         h         5         ARG           40         h         29         LYS           40         h         32         ARG           40         h         32         ARG           40         h         32         ARG           40         h         35         LYS           40         h         35         LYS           40         h         43         PHE           40         h         59         LEU           40         h         68         ASN           40         h         68         ASN           40         h         103         TRP           40         h         103         TRP           40         h         113         GLU           40         h         151         TYR           40         h         155         ARG           41         i         1         MET           41         i         1         MET           41         i         31	39	g	91	VAL
40         h         4         ARG           40         h         5         ARG           40         h         16         LEU           40         h         29         LYS           40         h         32         ARG           40         h         32         ARG           40         h         35         LYS           40         h         43         PHE           40         h         59         LEU           40         h         64         GLN           40         h         64         ASN           40         h         68         ASN           40         h         103         TRP           40         h         103         TRP           40         h         105         VAL           40         h         151         TYR           40         h         155         ARG           41         i         2         LEU           41         i         17         THR           41         i         17         THR           41         i         39	39	g	100	ASN
40         h         5         ARG           40         h         16         LEU           40         h         29         LYS           40         h         32         ARG           40         h         32         ARG           40         h         35         LYS           40         h         43         PHE           40         h         59         LEU           40         h         64         GLN           40         h         68         ASN           40         h         68         ASN           40         h         103         TRP           40         h         103         TRP           40         h         113         GLU           40         h         113         GLU           40         h         151         TYR           40         h         155         ARG           41         i         1         MET           41         i         1         MET           41         i         1         TYR           41         i         39	40	h	4	ARG
40         h         16         LEU           40         h         29         LYS           40         h         32         ARG           40         h         35         LYS           40         h         43         PHE           40         h         43         PHE           40         h         59         LEU           40         h         64         GLN           40         h         68         ASN           40         h         84         ASN           40         h         103         TRP           40         h         103         TRP           40         h         103         TRP           40         h         113         GLU           40         h         155         ARG           41         i         1         MET           41         i         2         LEU           41         i         17         THR           41         i         24         THR           41         i         39         LEU           41         i         3	40	h	5	ARG
40         h         29         LYS           40         h         32         ARG           40         h         35         LYS           40         h         43         PHE           40         h         43         PHE           40         h         59         LEU           40         h         64         GLN           40         h         68         ASN           40         h         84         ASN           40         h         103         TRP           40         h         103         TRP           40         h         103         TRP           40         h         105         VAL           40         h         113         GLU           40         h         155         ARG           41         i         1         MET           41         i         2         LEU           41         i         1         MET           41         i         24         THR           41         i         39         LEU           41         i         3	40	h	16	LEU
40         h         32         ARG           40         h         35         LYS           40         h         41         ARG           40         h         43         PHE           40         h         43         PHE           40         h         59         LEU           40         h         64         GLN           40         h         68         ASN           40         h         84         ASN           40         h         103         TRP           40         h         103         TRP           40         h         103         TRP           40         h         105         VAL           40         h         113         GLU           40         h         155         ARG           41         i         2         LEU           41         i         1         MET           41         i         2         LEU           41         i         17         THR           41         i         39         LEU           41         i         3	40	h	29	LYS
40         h         35         LYS           40         h         41         ARG           40         h         43         PHE           40         h         59         LEU           40         h         64         GLN           40         h         64         GLN           40         h         68         ASN           40         h         84         ASN           40         h         103         TRP           40         h         103         TRP           40         h         105         VAL           40         h         113         GLU           40         h         155         ARG           40         h         155         ARG           41         i         2         LEU           41         i         1         MET           41         i         21         LYS           41         i         21         LYS           41         i         31         PHE           41         i         39         LEU           41         i	40	h	32	ARG
40       h       41       ARG         40       h       43       PHE         40       h       59       LEU         40       h       64       GLN         40       h       68       ASN         40       h       84       ASN         40       h       103       TRP         40       h       103       TRP         40       h       105       VAL         40       h       113       GLU         40       h       151       TYR         40       h       155       ARG         40       h       155       ARG         41       i       2       LEU         41       i       1       MET         41       i       1       MET         41       i       21       LYS         41       i       24       THR         41       i       31       PHE         41       i       39       LEU         41       i       39       LEU         41       i       50       ARG         41	40	h	35	LYS
40         h         43         PHE           40         h         59         LEU           40         h         64         GLN           40         h         68         ASN           40         h         84         ASN           40         h         103         TRP           40         h         103         TRP           40         h         103         GLU           40         h         113         GLU           40         h         151         TYR           40         h         155         ARG           41         i         2         LEU           41         i         1         MET           41         i         2         LEU           41         i         1         MET           41         i         2         LEU           41         i         1         MET           41         i         21         LYS           41         i         39         LEU           41         i         39         LEU           41         i         50 </td <td>40</td> <td>h</td> <td>41</td> <td>ARG</td>	40	h	41	ARG
40         h         59         LEU           40         h         64         GLN           40         h         68         ASN           40         h         84         ASN           40         h         84         ASN           40         h         103         TRP           40         h         103         TRP           40         h         105         VAL           40         h         113         GLU           40         h         151         TYR           40         h         155         ARG           41         i         1         MET           41         i         1         MET           41         i         1         MET           41         i         2         LEU           41         i         1         MET           41         i         21         LYS           41         i         31         PHE           41         i         39         LEU           41         i         50         ARG           41         i         52<	40	h	43	PHE
40         h         64         GLN           40         h         68         ASN           40         h         84         ASN           40         h         103         TRP           40         h         103         TRP           40         h         103         TRP           40         h         103         VAL           40         h         113         GLU           40         h         151         TYR           40         h         151         TYR           40         h         155         ARG           41         i         2         LEU           41         i         2         LEU           41         i         14         ARG           41         i         21         LYS           41         i         24         THR           41         i         39         LEU           41         i         39         LEU           41         i         50         ARG           41         i         52         ASP           41         i <t< td=""><td>40</td><td>h</td><td>59</td><td>LEU</td></t<>	40	h	59	LEU
40         h         68         ASN           40         h         84         ASN           40         h         103         TRP           40         h         103         TRP           40         h         103         TRP           40         h         103         VAL           40         h         105         VAL           40         h         113         GLU           40         h         155         VARG           40         h         155         ARG           41         i         1         MET           41         i         2         LEU           41         i         14         ARG           41         i         21         LYS           41         i         21         LYS           41         i         39         LEU           41         i         39         LEU           41         i         50         ARG           41         i         52         ASP           41         i         52         ASP           41         i         <	40	h	64	GLN
40       h       84       ASN         40       h       103       TRP         40       h       103       TRP         40       h       105       VAL         40       h       113       GLU         40       h       113       GLU         40       h       151       TYR         40       h       155       ARG         40       h       155       ARG         41       i       1       MET         41       i       2       LEU         41       i       14       ARG         41       i       21       LYS         41       i       21       LYS         41       i       31       PHE         41       i       39       LEU         41       i       39       LEU         41       i       50       ARG         41       i       52       ASP         41       i       52       ASP         41       i       62       TYR         41       i       75       ARG         41	40	h	68	ASN
40       h       103       TRP         40       h       103       TRP         40       h       105       VAL         40       h       113       GLU         40       h       113       GLU         40       h       113       GLU         40       h       151       TYR         40       h       155       ARG         41       i       1       MET         41       i       2       LEU         41       i       14       ARG         41       i       17       THR         41       i       21       LYS         41       i       24       THR         41       i       39       LEU         41       i       39       LEU         41       i       45       ILE         41       i       50       ARG         41       i       52       ASP         41       i       52       ASP         41       i       62       TYR         41       i       85       ARG         41	40	h	84	ASN
40       h       105       VAL         40       h       113       GLU         40       h       113       GLU         40       h       113       GLU         40       h       151       TYR         40       h       151       TYR         40       h       155       ARG         41       i       1       MET         41       i       2       LEU         41       i       14       ARG         41       i       21       LYS         41       i       21       LYS         41       i       31       PHE         41       i       39       LEU         41       i       39       LEU         41       i       45       ILE         41       i       50       ARG         41       i       52       ASP         41       i       52       ASP         41       i       62       TYR         41       i       85       ARG         41       i       98       LYS         41	40	h	103	TRP
40       h       113       GLU         40       h       113       GLU         40       h       113       GLU         40       h       151       TYR         40       h       155       ARG         41       i       1       MET         41       i       2       LEU         41       i       14       ARG         41       i       2       LEU         41       i       14       ARG         41       i       21       LYS         41       i       21       LYS         41       i       31       PHE         41       i       39       LEU         41       i       39       LEU         41       i       45       ILE         41       i       50       ARG         41       i       52       ASP         41       i       62       TYR         41       i       75       ARG         41       i       98       LYS         41       i       99       GLU         41	40	h	105	VAL
40h $119$ ARG $40$ h $151$ TYR $40$ h $155$ ARG $41$ i1MET $41$ i2LEU $41$ i14ARG $41$ i17THR $41$ i21LYS $41$ i24THR $41$ i31PHE $41$ i39LEU $41$ i45ILE $41$ i50ARG $41$ i52ASP $41$ i62TYR $41$ i85ARG $41$ i98LYS $41$ i99GLU $41$ i103VAL	40	h	113	GLU
40h $151$ TYR $40$ h $155$ ARG $41$ i1MET $41$ i2LEU $41$ i14ARG $41$ i17THR $41$ i21LYS $41$ i24THR $41$ i39LEU $41$ i39LEU $41$ i50ARG $41$ i52ASP $41$ i52ASP $41$ i75ARG $41$ i85ARG $41$ i98LYS $41$ i99GLU $41$ i103VAL	40	h	119	ARG
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	40	h	151	TYR
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	40	h	155	ARG
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	41	i	1	MET
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	41	i	2	LEU
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	41	i	14	ARG
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	41	i	17	THR
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	41	i	21	LYS
41       i       31       PHE         41       i       39       LEU         41       i       45       ILE         41       i       45       ILE         41       i       50       ARG         41       i       52       ASP         41       i       62       TYR         41       i       75       ARG         41       i       85       ARG         41       i       98       LYS         41       i       99       GLU         41       i       103       VAL	41	i	24	THR
41       i       39       LEU         41       i       45       ILE         41       i       48       TYR         41       i       50       ARG         41       i       52       ASP         41       i       62       TYR         41       i       75       ARG         41       i       98       LYS         41       i       99       GLU         41       i       103       VAL	41	i	31	PHE
41       i       45       ILE         41       i       48       TYR         41       i       50       ARG         41       i       52       ASP         41       i       62       TYR         41       i       75       ARG         41       i       85       ARG         41       i       98       LYS         41       i       103       VAL	41	i	39	LEU
41       i       48       TYR         41       i       50       ARG         41       i       52       ASP         41       i       62       TYR         41       i       75       ARG         41       i       85       ARG         41       i       98       LYS         41       i       103       VAL	41	i	45	ILE
41       i       50       ARG         41       i       52       ASP         41       i       62       TYR         41       i       75       ARG         41       i       85       ARG         41       i       98       LYS         41       i       103       VAL	41	i	48	TYR
41         i         52         ASP           41         i         62         TYR           41         i         75         ARG           41         i         85         ARG           41         i         98         LYS           41         i         103         VAL	41	i	50	ARG
41       i       62       TYR         41       i       75       ARG         41       i       85       ARG         41       i       98       LYS         41       i       99       GLU         41       i       103       VAL	41	i	52	ASP
41         i         75         ARG           41         i         85         ARG           41         i         98         LYS           41         i         99         GLU           41         i         103         VAL	41	i	62	TYR
41         i         85         ARG           41         i         98         LYS           41         i         99         GLU           41         i         103         VAL	41	i	75	ARG
41         i         98         LYS           41         i         99         GLU           41         i         103         VAL	41	i	85	ARG
41         i         99         GLU           41         i         103         VAL	41	i	98	LYS
41 i 103 VAL	41	i	99	GLU
	41	i	103	VAL



Mol	Chain	Res	Type
41	i	104	ARG
41	i	105	ARG
41	i	107	LEU
41	i	122	ARG
41	i	127	LEU
42	j	5	TYR
42	j	53	VAL
42	j	85	LEU
42	j	89	ASN
42	j	92	TYR
42	j	108	VAL
42	j	114	TYR
42	j	125	TYR
42	j	127	LYS
43	k	8	LEU
43	k	11	PHE
43	k	46	ARG
43	k	47	PHE
43	k	49	VAL
43	k	57	LYS
43	k	61	GLU
43	k	64	GLU
43	k	65	LEU
43	k	71	LEU
43	k	79	ARG
43	k	82	ILE
44	1	20	TYR
44	1	29	ILE
44	1	33	THR
44	1	34	ASP
44	1	41	THR
44	1	51	LYS
44	1	73	MET
44	1	84	VAL
44	1	99	GLN
44	1	104	GLN
45	m	6	ILE
45	m	14	ARG
45	m	17	VAL
45	m	23	VAL
45	m	27	LYS
45	m	40	ARG



Mol	Chain	Res	Type
45	m	45	LYS
45	m	51	LEU
45	m	52	ARG
45	m	53	LYS
45	m	58	ARG
45	m	64	GLU
45	m	76	LEU
45	m	77	GLN
45	m	81	VAL
45	m	84	ILE
45	m	85	ARG
45	m	101	ARG
45	m	111	ASP
45	m	112	ARG
45	m	114	LYS
45	m	115	SER
45	m	121	THR
45	m	126	GLU
46	n	15	VAL
46	n	16	ASP
46	n	23	TYR
46	n	25	ILE
46	n	59	TYR
46	n	62	ASN
46	n	64	TRP
46	n	66	LEU
46	n	69	GLU
46	n	70	LEU
46	n	73	GLU
46	n	82	MET
46	n	86	CYS
46	n	91	ARG
46	n	92	HIS
46	n	93	ARG
46	n	94	ARG
46	n	98	VAL
46	n	99	ARG
46	n	103	THR
46	n	104	ARG
46	n	105	THR
46	n	108	ARG
46	n	120	LYS



Mol	Chain	Res	Type
46	n	125	ARG
47	0	8	GLU
47	0	11	LYS
47	0	16	PHE
47	0	21	TYR
47	0	24	CYS
47	0	29	ARG
47	0	33	VAL
47	0	36	PHE
47	0	41	ARG
47	0	42	ILE
47	0	49	HIS
47	0	56	VAL
48	р	6	GLU
48	p	8	LYS
48	p	26	GLU
48	p	32	LEU
48	p	35	ARG
48	p	54	ARG
48	p	56	LEU
48	р	57	LEU
48	p	67	LEU
48	р	69	TYR
48	р	71	GLN
48	р	83	GLU
48	р	84	LYS
49	q	1	MET
49	q	13	HIS
49	q	27	LYS
49	q	32	TYR
49	q	35	LYS
49	q	41	PRO
49	q	43	LYS
49	q	44	THR
49	q	48	TRP
49	q	52	ASP
49	q	58	TYR
49	q	60	LEU
49	q	71	ARG
49	q	74	LEU
49	q	79	VAL
50	r	6	LEU



Mol	Chain	Res	Type
50	r	14	LYS
50	r	17	LYS
50	r	19	VAL
50	r	36	ILE
50	r	41	LYS
50	r	42	TYR
50	r	43	LEU
50	r	55	ASP
50	r	58	GLU
50	r	69	LYS
50	r	72	ARG
50	r	81	ARG
50	r	84	LEU
50	r	88	TYR
50	r	94	ASN
50	r	100	LYS
51	S	13	GLN
51	S	29	PHE
51	S	31	LEU
51	s	32	ARG
51	S	33	ASP
51	S	34	TYR
51	S	42	ARG
51	S	63	GLN
52	t	6	LYS
52	t	23	ASN
52	t	25	LYS
52	t	29	ARG
52	t	31	ILE
52	t	32	LYS
52	t	33	THR
52	t	34	TRP
52	t	36	ARG
52	t	43	GLU
52	t	44	MET
52	t	49	ILE
52	t	53	ASN
52	t	55	LYS
52	t	60	VAL
52	t	61	TYR
52	t	63	THR
50	t	66	MET



$\mathbf{Mol}$	Chain	$\mathbf{Res}$	Type
52	t	71	LEU
53	u	10	LEU
53	u	20	LEU
53	u	21	LYS
53	u	23	ARG
53	u	27	LYS
53	u	51	GLU
53	u	53	LEU
53	u	56	MET
53	u	72	LEU
53	u	79	ARG
54	V	6	ARG
$\overline{54}$	V	9	ARG
54	V	14	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (134) such sidechains are listed below:

Mol	Chain	Res	Type
3	А	18	ASN
3	А	58	ASN
4	В	46	GLN
4	В	87	ASN
4	В	115	GLN
4	В	129	ASN
4	В	164	GLN
4	В	166	GLN
4	В	198	ASN
4	В	201	HIS
4	В	231	HIS
4	В	253	GLN
5	С	54	GLN
5	С	55	ASN
5	С	66	HIS
5	С	132	HIS
5	С	143	ASN
6	D	35	GLN
6	D	128	ASN
6	D	177	ASN
7	Е	40	ASN
7	Е	41	GLN
7	Е	66	GLN
7	Е	79	ASN



Mol	Chain	Res	Type
7	Е	123	ASN
8	F	61	HIS
8	F	65	HIS
8	F	74	ASN
8	F	143	GLN
9	G	28	ASN
9	G	43	ASN
9	G	104	GLN
9	G	147	GLN
10	Н	92	GLN
10	Н	124	HIS
11	Ι	3	GLN
11	Ι	29	ASN
12	J	9	ASN
12	J	38	GLN
12	J	81	GLN
13	K	12	GLN
13	Κ	45	GLN
13	K	46	GLN
13	K	57	HIS
13	K	123	HIS
14	L	16	HIS
14	L	23	ASN
14	L	71	GLN
15	М	38	GLN
16	Ν	38	ASN
16	Ν	90	GLN
17	0	44	ASN
17	0	72	HIS
18	Р	64	HIS
18	Р	87	HIS
19	Q	57	ASN
20	R	41	ASN
21	S	57	GLN
22	Т	34	ASN
22	Т	55	HIS
22	Т	65	GLN
22	Т	73	GLN
22	Т	75	ASN
23	U	35	ASN
23	U	40	GLN
23	U	80	HIS



Mol	Chain	Res	Type
24	V	19	GLN
24	V	45	ASN
25	W	47	ASN
26	Х	32	GLN
28	Ζ	16	HIS
29	a	35	GLN
35	с	25	ASN
35	с	78	GLN
35	с	94	ASN
35	с	135	GLN
35	с	204	ASN
36	d	3	ASN
36	d	6	HIS
36	d	28	GLN
36	d	63	ASN
36	d	102	ASN
36	d	110	ASN
36	d	118	GLN
36	d	136	GLN
36	d	139	GLN
37	е	45	GLN
37	е	74	GLN
37	е	77	ASN
37	е	119	GLN
37	е	129	ASN
37	е	199	ASN
37	е	201	GLN
38	f	20	GLN
38	f	65	ASN
38	f	72	GLN
39	g	18	GLN
39	g	27	GLN
39	g	32	ASN
39	g	94	GLN
40	h	13	GLN
40	h	64	GLN
40	h	68	ASN
40	h	84	ASN
40	h	86	GLN
40	h	97	GLN
40	h	106	GLN
40	h	109	ASN



Mol	Chain	Res	Type
40	h	110	GLN
40	h	122	HIS
41	i	15	ASN
41	i	70	GLN
42	j	73	GLN
42	j	89	ASN
43	k	56	HIS
43	k	76	ASN
44	1	27	ASN
44	1	38	ASN
45	m	7	ASN
45	m	77	GLN
46	n	40	ASN
46	n	101	GLN
47	0	49	HIS
48	р	13	GLN
48	р	37	ASN
48	р	42	HIS
48	р	62	GLN
49	q	16	HIS
49	q	76	GLN
50	r	26	GLN
51	s	63	GLN
52	t	47	HIS
53	u	26	ASN
53	u	42	GLN

## 5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	W	2888/2889~(99%)	983 (34%)	0
2	Х	119/120~(99%)	47 (39%)	0
31	У	1511/1522~(99%)	507~(33%)	0
32	Z	76/77~(98%)	20 (26%)	0
33	2	75/76~(98%)	22 (29%)	0
34	3	17/18~(94%)	5(29%)	0
All	All	4686/4702 (99%)	1584 (33%)	0

All (1584) RNA backbone outliers are listed below:



Mol	Chain	$\operatorname{Res}$	Type
1	W	10	G
1	W	13	А
1	W	15	G
1	W	27	G
1	W	28	А
1	W	29	U
1	W	34	С
1	W	35	G
1	W	37	С
1	W	43	G
1	W	46	С
1	W	49	А
1	W	50	U
1	W	51	G
1	W	52	А
1	W	61	G
1	W	64	А
1	W	69	С
1	W	71	А
1	W	72	U
1	W	73	А
1	W	75	G
1	W	78	А
1	W	83	G
1	W	88	G
1	W	89	G
1	W	90	U
1	W	92	G
1	W	95	G
1	W	96	G
1	W	101	G
1	W	102	G
1	W	103	А
1	W	117	G
1	W	118	А
1	W	119	А
1	W	120	U
1	W	121	G
1	W	125	G
1	W	126	А
1	W	131	G
1	W	137(A)	С
1	W	139	G
	<u>a</u>	7	



Mol	Chain	Res	Type
1	W	143	C
1	W	144	С
1	W	146	G
1	W	149	А
1	W	151	С
1	W	153	С
1	W	162	U
1	W	163	U
1	W	165	U
1	W	174	С
1	W	175	G
1	W	176	G
1	W	177	G
1	W	182	А
1	W	184	С
1	W	196	А
1	W	199	А
1	W	204	А
1	W	205	G
1	W	206	U
1	W	215	G
1	W	216	А
1	W	221	А
1	W	222	А
1	W	228	А
1	W	229	А
1	W	233	А
1	W	239	U
1	W	241	А
1	W	242	G
1	W	248	G
1	W	249	С
1	W	250	G
1	W	252	G
1	W	265	A
1	W	266	G
1	W	269	U
1	W	270(D)	С
1	W	270(E)	С
1	W	270(F)	G
1	W	270(M)	U
1	W	270(S)	G



Mol	Chain	Res	Type
1	W	270(T)	G
1	W	271(A)	U
1	W	271(B)	С
1	W	271(C)	G
1	W	271(D)	U
1	W	271	G
1	W	273(C)	С
1	W	273(G)	С
1	W	274	G
1	W	275	G
1	W	278	А
1	W	289	А
1	W	294	A
1	W	296	C
1	W	298	G
1	W	299	A
1	W	301	G
1	W	302	С
1	W	308	G
1	W	310	А
1	W	311	А
1	W	316	С
1	W	317	G
1	W	320	А
1	W	327	G
1	W	329	G
1	W	330	А
1	W	331	А
1	W	332	А
1	W	338	G
1	W	339	U
1	W	341	G
1	W	342	G
1	W	344	G
1	W	347	A
1	W	348	G
1	W	349	G
1	W	355	G
1	W	358	U
1	W	363(A)	G
1	W	363(E)	G
1	W	363(F)	U



Mol	Chain	Res	Type
1	W	364	С
1	W	366(B)	С
1	W	370	G
1	W	371	А
1	W	372	G
1	W	374	А
1	W	375	С
1	W	380	U
1	W	385	С
1	W	387	U
1	W	388	G
1	W	390	А
1	W	391	G
1	W	392	C
1	W	394	А
1	W	395	U
1	W	396	G
1	W	397	G
1	W	405	U
1	W	408	G
1	W	414	С
1	W	428	А
1	W	438	G
1	W	439	G
1	W	440	G
1	W	444	С
1	W	446	G
1	W	449	А
1	W	450	G
1	W	451	С
1	W	456	С
1	W	457	А
1	W	458	G
1	W	464	U
1	W	469	G
1	W	470	A
1	W	473	G
1	W	475	U
1	W	477	A
1	W	478	A
1	W	480	A
1	W	481	G
	Continu	ed on next	t page



1 1 1 1 1 1 1	W W W W	483 488 489	A G C
1 1 1 1 1 1	W W W	488 489	G
1 1 1 1	W W	489	С
1 1 1	W	401	U
1		491	G
1	W	492	А
-	W	504	U
1	W	505	А
1	W	508	G
1	W	509	С
1	W	510	С
1	W	517	С
1	W	518	G
1	W	522	G
1	W	527	С
1	W	528	А
1	W	529	A
1	W	531	С
1	W	532	А
1	W	533	G
1	W	537	С
1	W	542	С
1	W	544	С
1	W	549	G
1	W	551	G
1	W	556	G
1	W	559	G
1	W	562	U
1	W	563	G
1	W	567	А
1	W	569	U
1	W	572	A
1	W	573	G
1	W	574	С
1	W	575	A
1	W	583	G
1	W	594	U
1	W	595	С
1	W	598	G
1	W	603	A
1	W	604	G
1	W	610	С
1	W	614	U



Mol	Chain	Res	Type
1	W	615	G
1	W	616	А
1	W	617	G
1	W	618(B)	С
1	W	620	G
1	W	621	А
1	W	627	А
1	W	628	G
1	W	634	С
1	W	638	G
1	W	640	С
1	W	645	С
1	W	646	А
1	W	647	G
1	W	653	С
1	W	654	U
1	W	656	G
1	W	660	G
1	W	666	G
1	W	669	G
1	W	671	С
1	W	672	С
1	W	674	G
1	W	684	G
1	W	686	G
1	W	701	G
1	W	703	U
1	W	715	G
1	W	716	А
1	W	717	G
1	W	719	С
1	W	722	А
1	W	729	G
1	W	730	С
1	W	739	G
1	W	740	U
1	W	747	U
1	W	748	G
1	W	749	C
1	W	751	A
1	W	753	C
1	W	757	U
	Continu	ied on next	t page



Mol	Chain	Res	Type
1	W	763	G
1	W	764	А
1	W	765	G
1	W	770	G
1	W	775	G
1	W	776	G
1	W	781	A
1	W	782	А
1	W	784	А
1	W	789	А
1	W	790	С
1	W	792	G
1	W	794	G
1	W	796	С
1	W	798	G
1	W	800	A
1	W	805	G
1	W	811	U
1	W	812	С
1	W	817	С
1	W	826	U
1	W	827	U
1	W	828	U
1	W	830	G
1	W	831	G
1	W	835	А
1	W	846	С
1	W	847	U
1	W	848	G
1	W	849	А
1	W	855	G
1	W	856	C
1	W	859	G
1	W	860	U
1	W	861	А
1	W	866	A
1	W	867	С
1	W	870	A
1	W	873	G
1	W	876	C
1	W	885	C
1	W	886	С



Mol	Chain	Res	Type
1	W	887	А
1	W	888	С
1	W	889	С
1	W	890	А
1	W	897	С
1	W	899	А
1	W	900	А
1	W	902	С
1	W	906	G
1	W	907	U
1	W	909	А
1	W	910	А
1	W	912	С
1	W	914	С
1	W	916	G
1	W	926	А
1	W	928	G
1	W	931	G
1	W	932	G
1	W	933	А
1	W	938	G
1	W	945	А
1	W	946	G
1	W	957	А
1	W	958	U
1	W	959	А
1	W	961	С
1	W	962	G
1	W	963	U
1	W	965	С
1	W	966	G
1	W	972	G
1	W	974(A)	G
1	W	974(B)	С
1	W	975	G
1	W	976	С
1	W	977	G
1	W	980	A
1	W	982	С
1	W	983	A
1	W	989	G
1	W	990	A
	<u> </u>	1	



Mol	Chain	Res	Type
1	W	991	С
1	W	992	С
1	W	993	G
1	W	996	А
1	W	997	G
1	W	1006	С
1	W	1008	С
1	W	1009	А
1	W	1011	G
1	W	1012	U
1	W	1013	С
1	W	1015	G
1	W	1016	G
1	W	1017	G
1	W	1020	А
1	W	1021	А
1	W	1022	G
1	W	1023	U
1	W	1025	G
1	W	1026	U
1	W	1033	U
1	W	1034	G
1	W	1042	G
1	W	1043	С
1	W	1045	А
1	W	1046	А
1	W	1047	G
1	W	1054	А
1	W	1059	G
1	W	1060	U
1	W	1061	U
1	W	1062	G
1	W	1070	А
1	W	1071	G
1	W	1072	С
1	W	1079	С
1	W	1080	С
1	W	1083	U
1	W	1087	G
1	W	1088	А
1	W	1089	G
1	W	1111	А
	Continu	ed on next	page



Mol	Chain	Res	Type
1	W	1112	G
1	W	1126	А
1	W	1129	А
1	W	1130	U
1	W	1131	G
1	W	1132	А
1	W	1135	С
1	W	1136	G
1	W	1139	G
1	W	1141	U
1	W	1142	С
1	W	1142(B)	А
1	W	1143	А
1	W	1144	G
1	W	1148	А
1	W	1152	С
1	W	1155	А
1	W	1157	G
1	W	1161	С
1	W	1166	С
1	W	1170	G
1	W	1175	U
1	W	1177	А
1	W	1179	С
1	W	1180	С
1	W	1182	А
1	W	1183	G
1	W	1186	G
1	W	1187	G
1	W	1188	U
1	W	1191	G
1	W	1194	А
1	W	1195	G
1	W	1197	G
1	W	1199	U
1	W	1200	C
1	W	1201	C
1	W	1202	C
1	W	1204	A
1	W	1205	U
1	W	1208	С
1	W	1210	A



Mol	Chain	Res	Type
1	W	1211	U
1	W	1212	G
1	W	1220	А
1	W	1221	С
1	W	1224	С
1	W	1227	G
1	W	1229	G
1	W	1237	А
1	W	1238	G
1	W	1240	U
1	W	1244	G
1	W	1247	А
1	W	1248	G
1	W	1250	G
1	W	1251	С
1	W	1252	G
1	W	1253	А
1	W	1256	G
1	W	1265	А
1	W	1266	G
1	W	1267	U
1	W	1271	G
1	W	1272	А
1	W	1273	U
1	W	1274	А
1	W	1275	А
1	W	1276	А
1	W	1278	А
1	W	1280	G
1	W	1289	С
1	W	1295	С
1	W	1296	G
1	W	1298	С
1	W	1300	U
1	W	1301	А
1	W	1302	А
1	W	1305	С
1	W	1310	G
1	W	1313	U
1	W	1320	С
1	W	1321	А
1	W	1325	G
	Continu	ed on next	page



Mol	Chain	Res	
1	W	1326	U
1	W	1329	U
1	W	1339	G
1	W	1341	U
1	W	1343	G
1	W	1347	G
1	W	1359	A
1	W	1360	A
1	W	1362	C
1	W	1365	A
1	W	1366	A
1	W	1368	G
1	W	1378	A
1	W	1379	A
1	W	1384	A
1	W	1385	G
1	W	1305	
1	W	1308	
1	VV XX7	1/16	C
1	W	1410	G A
1	W	1419	
1	W	1420	
1	W	1420	G
1	W	1427	A C
1	W	1420	
1	W	1404	A C
1	W	1430	G U
1	W	1438	
1	W	1444(B) 1445	A
1	W	1440	C
1	W	1440	G
1	W	1448(B)	A
1	W	1449	G
1	W	1451	
1	W	1453	A
1	W	1454	
1	W	1455	G
1	W	1458	C
1	W	1459	G
1	W	1460	A
1	W	1461	G
1	W	1467	C
1	W	1471	A



Mol	Chain	Res	Type
1	W	1472	А
1	W	1478	G
1	W	1479	G
1	W	1481	U
1	W	1483	G
1	W	1485	G
1	W	1487	G
1	W	1488	G
1	W	1490	А
1	W	1491	G
1	W	1497	U
1	W	1498	С
1	W	1502	С
1	W	1506	С
1	W	1508	А
1	W	1509	А
1	W	1510	А
1	W	1517	G
1	W	1519	G
1	W	1520	U
1	W	1521	G
1	W	1522	G
1	W	1535	U
1	W	1536	А
1	W	1537	С
1	W	1538	G
1	W	1540	G
1	W	1543	А
1	W	1544	С
1	W	1545	А
1	W	1546(B)	С
1	W	1547	С
1	W	1555	G
1	W	1558	А
1	W	1559	G
1	W	1560	G
1	W	1567	А
1	W	1569	A
1	W	1570	A
1	W	1576	U
			<i><i><i></i></i></i>
1	W	1577	C



Mol	Chain	Res	Type
1	W	1579	A
1	W	1581	G
1	W	1585	С
1	W	1586	A
1	W	1595	G
1	W	1596	А
1	W	1603	А
1	W	1607	С
1	W	1608	А
1	W	1609	А
1	W	1610	А
1	W	1613	G
1	W	1616	А
1	W	1617	С
1	W	1618	А
1	W	1619	G
1	W	1626	G
1	W	1628	G
1	W	1634	А
1	W	1635	G
1	W	1639	U
1	W	1640	С
1	W	1642	G
1	W	1646	С
1	W	1647	G
1	W	1648	С
1	W	1654	А
1	W	1664	А
1	W	1669	А
1	W	1670	С
1	W	1672	С
1	W	1674	G
1	W	1682	G
1	W	1688	U
1	W	1693	U
1	W	1694	С
1	W	1699	G
1	W	1700	A
1	W	1703	G
1	W	1707	G
1	W	1717	G
1	W	1718	G



Mol	Chain	Res	Type
1	W	1731	G
1	W	1733	G
1	W	1742	С
1	W	1743	G
1	W	1747	G
1	W	1748	G
1	W	1754	С
1	W	1756	G
1	W	1758	G
1	W	1759	А
1	W	1763	G
1	W	1764	G
1	W	1773	А
1	W	1777	U
1	W	1780	А
1	W	1781	С
1	W	1782	С
1	W	1785	А
1	W	1787	А
1	W	1792	G
1	W	1800	С
1	W	1801	G
1	W	1802	А
1	W	1806	С
1	W	1810	А
1	W	1815	А
1	W	1816	G
1	W	1817	G
1	W	1818	U
1	W	1819	А
1	W	1820	U
1	W	1821	А
1	W	1823	G
1	W	1824	G
1	W	1825	А
1	W	1829	A
1	W	1836	C
1	W	1838	C
1	W	1839	G
1	W	1843	C
1	W	1847	A
1	W	1858	G



1 1	W	1850	
1		1000	A
	W	1863	G
1	W	1864	U
1	W	1869	G
1	W	1878	G
1	W	1879	С
1	W	1885	А
1	W	1886	С
1	W	1888	G
1	W	1889	А
1	W	1900	А
1	W	1903	G
1	W	1906	G
1	W	1912	A
1	W	1913	А
1	W	1914	С
1	W	1915	U
1	W	1916	А
1	W	1929	G
1	W	1930	G
1	W	1935	G
1	W	1936	А
1	W	1937	А
1	W	1938	А
1	W	1939	U
1	W	1944	U
1	W	1955	U
1	W	1956	U
1	W	1960	А
1	W	1963	U
1	W	1964	G
1	W	1965	С
1	W	1966	A
1	W	1967	С
1	W	1968	G
1	W	1969	A
1	W	1971	A
1	W	1972	A
1	W	1982	С
1	W	1987	G
1	W	1991	U
1	W	1992	G



Mol	Chain	Res	Type
1	W	1993	U
1	W	1997	G
1	W	1998	G
1	W	2001	А
1	W	2010	G
1	W	2013	А
1	W	2014	А
1	W	2020	А
1	W	2023	G
1	W	2026	С
1	W	2031	А
1	W	2033	А
1	W	2035	G
1	W	2040	С
1	W	2041	U
1	W	2043	С
1	W	2050	С
1	W	2051	А
1	W	2052	G
1	W	2055	С
1	W	2056	G
1	W	2057	А
1	W	2059	А
1	W	2060	А
1	W	2061	G
1	W	2062	А
1	W	2063	С
1	W	2066	С
1	W	2067	G
1	W	2068	U
1	W	2069	G
1	W	2076	U
1	W	2077	А
1	W	2080	G
1	W	2087	G
1	W	2092	U
1	W	2093	G
1	W	2096	U
1	W	2099	U
1	W	2100	G
1	W	2110	G
1	W	2111	С
	Continu	ded on next	page



$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	G G U A G U
1         w         2116           1         w         2118           1         w         2119           1         w         2120           1         w         2122	G U A G U
1         w         2118           1         w         2119           1         w         2120           1         w         2122	U A G U
1         w         2119           1         w         2120           1         w         2122	A G U
$1  ext{ w}  ext{ 2120}$ 1	G U
1 w 9199	U
1 W 2122	
1 w 2124	G
1 w 2126	А
1 w 2127	G
1 w 2128	С
1 w 2129	С
1 w 2130	U
1 w 2131	G
1 w 2132	U
1 w 2133	G
1 w 2136	C
1 w 2138	С
1 w 2157	G
1 w 2158	А
1 w 2160	G
1 w 2169	А
1 w 2171	А
1 w 2172	U
1 w 2173	А
1 w 2174	С
1 w 2176	А
1 w 2177	С
1 w 2179	С
1 w 2181	G
1 w 2188	С
1 w 2190	G
1 w 2191	G
1 w 2192	G
1 w 2194	G
1 w 2195	С
1 w 2205	С
1 w 2211	G
1 w 2213	U
1 w 2215	G
1 w 2217	G
1 w 2225	А
1 w 2226	С



Mol	Chain	Res	Type
1	W	2238	G
1	W	2239	G
1	W	2243	U
1	W	2251	G
1	W	2257	U
1	W	2264	С
1	W	2269	А
1	W	2275	С
1	W	2276	G
1	W	2283	С
1	W	2287	А
1	W	2288	А
1	W	2290	G
1	W	2294	С
1	W	2297	С
1	W	2304	G
1	W	2305	А
1	W	2307	G
1	W	2308	G
1	W	2309	А
1	W	2310	А
1	W	2319	G
1	W	2320	А
1	W	2321	G
1	W	2323	G
1	W	2325	G
1	W	2327	А
1	W	2333	A
1	W	2334	G
1	W	2336	A
1	W	2344	U
1	W	2345	G
1	W	2346	A
1	W	2347	C
1	W	2350	С
1	W	2354	G
1	W	2356	C
1	W	2361	A
1	W	$236\overline{5}$	G
1	W	2368	С
1	W	2376	A
1	W	2377	А


Mol	Chain	Res	Type
1	W	2379	G
1	W	2382	G
1	W	2383	G
1	W	2385	С
1	W	2388	A
1	W	2391	G
1	W	2394	С
1	W	2398	U
1	W	2399	G
1	W	2400	G
1	W	2402	С
1	W	2406	U
1	W	2407	G
1	W	2422	A
1	W	2423	U
1	W	2425	A
1	W	2427	С
1	W	2428	G
1	W	2429	G
1	W	2430	А
1	W	2431	U
1	W	2432	A
1	W	2434	А
1	W	2435	А
1	W	2439	A
1	W	2441	С
1	W	2442	С
1	W	2447	G
1	W	2448	A
1	W	2449	U
1	W	2450	A
1	W	2452	С
1	W	2455	G
1	W	2469	A
1	W	2472	G
1	W	2478	A
1	W	2480	С
1	W	2483	С
1	W	2484	G
1	W	2487	G
1	W	2491	U
1	W	2498	С



Mol	Chain	Res	Type
1	W	2501	С
1	W	2502	G
1	W	2503	А
1	W	2504	U
1	W	2505	G
1	W	2506	U
1	W	2513	G
1	W	2514	U
1	W	2515	С
1	W	2516	G
1	W	2518	А
1	W	2519	U
1	W	2523	G
1	W	2529	G
1	W	2542	A
1	W	2543	G
1	W	2549	G
1	W	2551	С
1	W	2554	U
1	W	2555	U
1	W	2560	С
1	W	2563	U
1	W	2566	А
1	W	2567	G
1	W	2569	G
1	W	2572	А
1	W	2573	С
1	W	2574	G
1	W	2576	G
1	W	2578	G
1	W	2581	G
1	W	2582	G
1	W	2584	U
1	W	2588	G
1	W	2589	A
1	W	2590	A
1	W	2602	A
1	W	2606	C
1	W	2609	U
1	W	2611	U
1	W	2612	С
1	W	2615	U



Mal	Chain	Rog	Type
1	Unain 	10 <b>5</b>	гуре
1	W	2010	C
1	W	2018	G
1	W	2619	C
1	W	2621	A
1	W	2622	C
1	W	2628	С
1	W	2629	A
1	W	2630	G
1	W	2635	С
1	W	2637	U
1	W	2639	А
1	W	2642	G
1	W	2643	G
1	W	2645	G
1	W	2646	С
1	W	2647	U
1	W	2653	U
1	W	2654	А
1	W	2655	G
1	W	2656	U
1	W	2658	C
1	W	2665	A
1	W	2674	G
1	W	2681	C
1	W	2682	U
1	w	2602	C
1	W	2694	G
1	VV	2605	C
1	W	2095	U
1	w	2702	U
1	w	2112 9719(D)	
1	W	2(12(D))	A
1	W	2713	A
1	W	2(14	G
1	W	2718	G
1	W	2719	G
1	W	2720	U
1	W	2721	A
1	W	2722	G
1	W	2735	G
1	W	2739	U
1	W	2744	G
1	W	2746	U
	Continu	ed on next	page



G A
A
_
С
U
C
A
A
G
G
G
А
G
С
С
А
A
U
А
С
С
G
G
U
С
A
G
С
G
U
А
А
С
G
G
G
А
U
G
G
U
С
U



Mol	Chain	Res	Type
1	W	2866	U
1	W	2867	G
1	W	2868	А
1	W	2872	G
1	W	2873	A
1	W	2875	С
1	W	2876	G
1	W	2880	С
1	W	2883	A
1	W	2884	U
1	W	2887	U
1	W	2889	С
1	W	2892	A
1	W	2895	U
1	W	2896	С
1	W	2901	С
2	X	5	С
2	X	8	U
2	X	9	G
2	X	10	С
2	X	11	С
2	X	13	A
2	X	14	U
2	X	15	A
2	X	16	G
2	X	20	С
2	X	21	G
2	X	25	A
2	X	26	A
2	X	27	С
2	X	29	А
2	X	33	G
2	X	35	U
2	x	39	A
2	X	40	U
2	X	42	С
2	Х	43	С
2	X	45	A
2	X	49	С
2	x	50	G
2	X	52	А
2	X	53	А
	Continu	ed on nex	t page

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Mol	Chain	Res	Type
2	Х	54	G
2	Х	57	А
2	Х	64	С
2	Х	66	А
2	Х	67	G
2	Х	69	G
2	х	74	U
2	Х	75	G
2	Х	76	G
2	Х	79	С
2	Х	87	G
2	Х	90	С
2	Х	98	G
2	х	103	U
2	Х	107	U
2	х	108	С
2	Х	109	G
2	х	113	С
2	х	114	G
2	Х	117	G
2	Х	118	G
31	у	6	G
31	у	8	А
31	у	9	G
31	у	13	U
31	y	14	U
31	у	15	G
31	у	21	G
31	у	31	G
31	у	32	А
31	у	37	U
31	у	38	G
31	у	39	G
31	у	44	G
31	у	47	С
31	у	48	С
31	у	50	А
31	у	51	А
31	у	56	U
31	у	61	G
		CO	TT
31	У	62	U



Mol	Chain	Res	Type
31	у	69	G
31	y	82	U
31	y	93	U
31	y	95	G
31	y	97	U
31	y	99	С
31	y	104	G
31	y	105	G
31	y	110	С
31	y	112	G
31	у	115	G
31	у	116	А
31	у	120	А
31	у	121	С
31	у	122	G
31	у	129(B)	G
31	у	130	А
31	у	131	С
31	у	133	U
31	у	134	А
31	у	136	С
31	У	139	G
31	у	141	А
31	У	143	А
31	У	145	G
31	У	149	А
31	У	152	А
31	У	157	G
31	у	161	А
31	у	162	А
31	У	163	С
31	у	174	C
31	У	179	A
31	у	189	U
31	у	191(A)	G
31	У	195	А
31	у	196	А
31	у	197	A
31	у	198	G
31	У	208	U
31	У	209	U
0.1	1	010	TT



Mol	Chain	Res	Type
31	у	216	G
31	у	219	С
31	у	223	U
31	у	234	С
31	У	238	G
31	У	244	U
31	У	247	G
31	У	251	G
31	У	252	U
31	У	253	U
31	У	255	G
31	у	258	G
31	У	259	G
31	У	263	А
31	у	266	G
31	У	267	С
31	У	270	А
31	у	279	А
31	у	280	С
31	У	281	G
31	У	289	G
31	У	295	С
31	У	299	G
31	У	300	А
31	У	312	С
31	У	321	А
31	У	322	С
31	У	327	А
31	У	328	С
31	У	329	А
31	У	330	С
31	У	332	G
31	У	344	A
31	У	345	C
31	У	347	G
31	У	351	G
31	У	352	C
31	У	353	A
31	У	354	G
31	У	357	G
31	У	360	A
31	У	361	G



Mol	Chain	Res	Type
31	у	363	A
31	y	365	U
31	y	366	С
31	y	368	U
31	y	369	С
31	y	372	С
31	y	373	А
31	y	375	U
31	y	377	G
31	y	378	G
31	у	379	С
31	у	382	А
31	у	388	G
31	у	391	G
31	У	392	G
31	У	395	С
31	у	397	А
31	у	398	С
31	у	406	G
31	у	409	G
31	у	410	G
31	у	412	А
31	у	413	G
31	у	414	А
31	у	421	U
31	у	422	С
31	у	423	G
31	у	428	G
31	у	429	U
31	у	430	А
31	у	436	С
31	У	439	А
31	У	440	А
31	У	445	G
31	У	449	C
31	У	452	A
31	У	466	G
31	У	467	G
31	У	480	U
31	У	484	G
31	V	485	G
	y	100	~



Mol	Chain	Res	Type
31	у	491	G
31	y	493	G
31	y	496	А
31	y	497	U
31	y	498	А
31	y	500	G
31	y	506	G
31	y	508	С
31	y	509	А
31	у	511	С
31	y	512	U
31	y	513	С
31	y	516	PSU
31	y	517	G
31	y	518	С
31	y	519	С
31	y	521	G
31	y	523	А
31	y	524	G
31	y	525	С
31	y	527	7MG
31	y	529	G
31	y	531	U
31	y	532	А
31	y	533	А
31	y	543	С
31	y	547	А
31	у	549	С
31	у	552	U
31	у	556	С
31	у	557	G
31	у	560	U
31	у	561	U
31	у	562	С
31	у	563	А
31	у	565	U
31	у	566	G
31	у	570	G
31	у	572	А
31	у	573	А
31	у	575	G
31	у	576	G



Mol	Chain	Res	Type
31	у	577	G
31	y	585	G
31	y	588	G
31	y	611	А
31	y	616	G
31	y	617	G
31	y	619	U
31	y	623	С
31	y	627	G
31	y	630	G
31	у	631	G
31	у	633	G
31	у	641	U
31	у	643	С
31	У	650	G
31	у	652	U
31	у	653	А
31	у	661	G
31	у	672	U
31	у	673	G
31	у	678	U
31	У	687	А
31	у	688	G
31	У	689	С
31	У	693	G
31	У	697	U
31	У	701	С
31	У	702	А
31	у	703	G
31	у	704	А
31	У	705	U
31	У	718	G
31	У	724	G
31	у	725	G
31	У	733	A
31	У	741	G
31	У	747	С
31	У	748	С
31	у	749	С
31	У	750	G
31	V	752	G
	3		-



31 31 31 31	y v	755	G
31 31 31	v		· · · ·
31 31		759	A
31	v	770	С
-	v	771	G
31	v	772	U
31	v	777	А
31	v	781	А
31	v	792	А
31	y	794	А
31	y	796	С
31	y	800	G
31	y	801	U
31	y	809	G
31	y	813	U
31	y	814	А
31	y	815	А
31	y	816	А
31	y	817	С
31	y	818	G
31	y	820	U
31	y	828	А
31	y	833	U
31	y	841	U
31	у	842	С
31	y	843	U
31	y	848	С
31	у	852	G
31	у	863	U
31	у	870	U
31	у	871	U
31	у	872	А
31	у	873	А
31	у	874	G
31	у	876	G
31	у	885	G
31	у	889	А
31	у	890	G
31	у	900	А
31	у	902	G
31	у	905	U
31	у	910	С
31	у	913	А



Mol	Chain	Res	Type
31	у	914	A
31	y	916	G
31	y	926	G
31	v	927	G
31	y	928	G
31	y	934	С
31	y	936	С
31	y	939	G
31	y	942	G
31	y	947	G
31	y	948	С
31	y	956	U
31	y	958	A
31	y	960	U
31	y	961	U
31	y	964	A
31	y	965	А
31	у	966	M2G
31	у	967	5MC
31	у	968	А
31	у	969	А
31	у	972	С
31	у	974	А
31	У	975	А
31	у	976	G
31	у	977	А
31	У	978	А
31	У	982	U
31	У	983	А
31	У	991	U
31	У	992	U
31	у	993	G
31	у	995	С
31	у	998(A)	G
31	у	1002	G
31	У	1004	A
31	У	1005	A
31	У	1013	G
31	у	1014	A
31	у	1016	A
31	У	1020	U
31	У	1024	G



Mol	Chain	Res	Type
31	у	1025	U
31	у	1026	G
31	y	1027	С
31	y	102(A)	С
31	y	102(C)	С
31	у	1029	G
31	У	1030	С
31	y	1042	G
31	y	1050	G
31	y	1053	G
31	у	1054	С
31	y	1055	А
31	у	1062	U
31	у	1064	G
31	У	1065	U
31	у	1066	С
31	y	1068	G
31	у	1070	U
31	у	1078	U
31	y	1079	G
31	у	1080	А
31	у	1081	G
31	у	1085	U
31	у	1086	U
31	у	1089	G
31	у	1090	U
31	у	1094	G
31	У	1095	U
31	У	1101	А
31	У	1102	А
31	У	1104	G
31	У	1108	G
31	У	1109	С
31	У	1114	С
31	У	1118	С
31	У	1126	U
31	У	1127	G
31	У	1130	А
31	У	1136	U
31	У	1137	С
31	У	1139	G
31	У	1140	С



Mol	Chain	Res	Type
31	v	11/2	C C
31	y V	1143	G
31	y v	1140	G
31	y V	1144	
31	y v	1140	
31	y V	1154	C A
31	y V	1154	
31	y V	1157	
31 31	y V	1150	U
31 31	y V	1169	
21	y v	1102	
01 91	У	1107	A C
01 	<u>у</u>	1170	G
<u>ე1</u>	У	1170	A
31 	У	1170	G
ঠা 01	У	11/9	A
31 	У	1184	G
31	У	1188	A
31	У	1190	G
31	У	1196	U
31	У	1197	G
31	У	1198	G
31	У	1200	C
31	У	1202	G
31	У	1203	C
31	У	1207	2MG
31	У	1208	C
31	У	1209	С
31	У	1211	U
31	У	1212	U
31	У	1213	A
31	У	1215	G
31	У	1221	G
31	У	1225	A
31	у	1226	C
31	У	1227	A
31	У	$123\overline{3}$	G
31	У	1235	U
31	У	1237	С
31	у	1238	A
31	у	1239	A
31	У	1240	U
31	У	1241	G



Mol	Chain	Res	Type
31	у	1243	C
31	v	1247	U
31	y	1248	А
31	v	1251	А
31	y	1253	G
31	y	1256	А
31	y	1257	U
31	y	1261	А
31	y	1263	С
31	y	1267	С
31	у	1269	А
31	у	1270	С
31	у	1278	U
31	у	1280	А
31	У	1282	С
31	у	1283	G
31	У	1285	А
31	У	1286	А
31	У	1290	G
31	у	1291	G
31	у	1294	G
31	у	1297	С
31	у	1298	С
31	у	1299	А
31	у	1300	G
31	у	1301	U
31	у	1302	U
31	у	1303	С
31	у	1306	А
31	У	1308	U
31	У	1309	G
31	У	1319	А
31	У	1320	С
31	У	1323	G
31	У	1324	А
31	У	1325	С
31	У	1331	G
31	У	1333	A
31	У	1335	С
31	У	1340	A
31	У	1345	U
31	У	1346	A



Mol	Chain	Res	Type
31	у	1347	G
31	y	1348	U
31	y	1354	С
31	y	1359	С
31	y	1360	А
31	y	1361	G
31	y	136(B)	С
31	y	1363	А
31	y	1364	U
31	y	1365	G
31	у	1366	С
31	y	1369	С
31	у	1378	С
31	y	1380	U
31	y	1381	U
31	y	1388	С
31	y	1394	А
31	y	1396	А
31	y	1397	С
31	y	1398	А
31	y	1400	5MC
31	y	1401	G
31	y	1402	С
31	y	1404	5MC
31	y	1405	G
31	y	1407	5MC
31	y	1408	А
31	y	1420	С
31	y	1426	С
31	у	1434	А
31	у	1442	G
31	у	1443	G
31	у	1446	А
31	у	1447	G
31	у	1451	А
31	У	1452	С
31	У	1454	G
31	у	1468	А
31	у	1471	G
31	У	1472	U
		1475	C
31	У	1470	G



Mol	Chain	Res	Type
31	у	1490	С
31	у	1491	G
31	у	1492	А
31	у	1494	G
31	y	1495	U
31	у	1498	U
31	у	1501	С
31	у	1502	А
31	у	1504	G
31	У	1505	G
31	у	1506	U
31	У	1507	А
31	У	1513	А
31	У	1517	G
31	у	1520	G
31	У	1521	G
31	у	1525	G
31	У	1527	С
31	У	1529	G
31	У	1530	G
31	У	1531	А
31	у	1532	U
31	У	1534	А
31	У	1535	С
32	Z	9	G
32	Z	16	С
32	Z	17	С
32	Z	17(A)	U
32	Z	18	G
32	Z	19	G
32	Z	20	U
32	Z	21	A
32	Z	25	С
32	Z	26	G
32	Z	30	G
32	Z	35	A
32	Z	46	A
32	Z	48	C
32	Z	49	G
32	Z	59	A
32	Z	65	С
32	Z	71	C
	Continu	ied on next	t page



Mol	Chain	Res	Type
32	Z	73	А
32	Z	76	А
33	2	8	U
33	2	9	А
33	2	10	G
33	2	14	А
33	2	15	G
33	2	16	U
33	2	17	U
33	2	18	G
33	2	20	G
33	2	21	А
33	2	22	G
33	2	35	А
33	2	36	А
33	2	40	С
33	2	47	U
33	2	48	С
33	2	55	PSU
33	2	61	С
33	2	67	А
33	2	73	А
33	2	75	С
33	2	76	А
34	3	3	G
34	3	6	G
34	3	12	А
34	3	13	А
34	3	16	А

There are no RNA pucker outliers to report.

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

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

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



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Mal	Type	Chain	Dog	Link	Bo	Bond lengths			Bond angles		
WIOI	туре	Ullalli	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2	
31	MA6	У	1519	31	$19,\!26,\!27$	2.21	4 (21%)	18,38,41	1.89	5 (27%)	
31	M2G	У	966	31	20,27,28	1.63	4 (20%)	22,40,43	1.32	2 (9%)	
31	5MC	У	1400	31	18,22,23	0.95	1 (5%)	26,32,35	0.98	1 (3%)	
31	7MG	У	527	31	22,26,27	<mark>3.33</mark>	3 (13%)	29,39,42	1.69	6 (20%)	
31	5MC	У	1404	31	18,22,23	1.04	1 (5%)	26,32,35	1.48	4 (15%)	
33	PSU	2	55	33	18,21,22	1.81	3 (16%)	22,30,33	2.02	6 (27%)	
31	MA6	У	1518	31	19,26,27	1.79	2 (10%)	18,38,41	2.21	6 (33%)	
31	5MC	У	1407	31	18,22,23	0.87	1 (5%)	26,32,35	1.29	3 (11%)	
31	5MC	У	967	31	18,22,23	0.74	1 (5%)	26,32,35	1.28	3 (11%)	
31	PSU	У	516	31	18,21,22	2.00	5 (27%)	22,30,33	1.85	5 (22%)	
31	2MG	У	1207	31	18,26,27	1.88	4 (22%)	16,38,41	1.45	3 (18%)	

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
31	MA6	У	1519	31	-	3/7/29/30	0/3/3/3
31	M2G	У	966	31	-	0/7/29/30	0/3/3/3
31	5MC	у	1400	31	-	0/7/25/26	0/2/2/2
31	7MG	У	527	31	-	0/7/37/38	0/3/3/3
31	5MC	У	1404	31	-	2/7/25/26	0/2/2/2
33	PSU	2	55	33	-	4/7/25/26	0/2/2/2
31	MA6	У	1518	31	-	2/7/29/30	0/3/3/3
31	5MC	у	1407	31	-	0/7/25/26	0/2/2/2
31	5MC	У	967	31	-	0/7/25/26	0/2/2/2
31	PSU	у	516	31	-	0/7/25/26	0/2/2/2
31	2MG	У	1207	31	-	1/5/27/28	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
31	У	527	7MG	C8-N9	-14.62	1.37	1.46
31	у	1518	MA6	C6-N1	5.46	1.41	1.33
31	у	1519	MA6	O4'-C1'	5.27	1.48	1.41
33	2	55	PSU	O2-C2	5.19	1.34	1.23
31	У	1519	MA6	C6-N1	5.10	1.40	1.33
31	У	516	PSU	O2-C2	5.05	1.34	1.23



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	у	1207	2MG	C6-N1	4.93	1.45	1.37
31	у	516	PSU	C6-C5	4.55	1.40	1.35
31	у	966	M2G	C6-N1	4.33	1.44	1.37
33	2	55	PSU	C6-C5	4.11	1.40	1.35
31	у	1519	MA6	C10-N6	4.05	1.55	1.45
31	у	1207	2MG	C2-N1	4.02	1.43	1.36
33	2	55	PSU	C2-N1	2.91	1.40	1.36
31	у	1519	MA6	C9-N6	2.89	1.52	1.45
31	у	966	M2G	C2-N3	2.85	1.34	1.30
31	у	516	PSU	C2-N1	2.83	1.40	1.36
31	у	966	M2G	C2-N1	2.82	1.43	1.36
31	у	527	7MG	C6-N1	2.77	1.44	1.38
31	у	527	7MG	C5-N7	2.76	1.38	1.35
31	у	516	PSU	C2'-C1'	2.59	1.57	1.53
31	у	1404	5MC	C4-N4	2.58	1.40	1.34
31	у	1407	5MC	C4-N4	2.56	1.40	1.34
31	У	1400	5MC	C4-N4	2.51	1.40	1.34
31	У	967	5MC	C4-N4	2.30	1.40	1.34
31	у	1207	2MG	CM2-N2	2.28	1.49	1.45
31	У	1207	2MG	C8-N7	-2.17	1.31	1.35
31	у	1518	MA6	C2-N3	2.07	1.35	1.32
31	У	516	PSU	O4'-C1'	2.06	1.46	1.43
31	У	966	M2G	C8-N7	-2.03	1.31	1.35

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All	(44)	bond	angle	outliers	are	listed	below:
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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
31	у	527	7MG	N9-C8-N7	6.33	112.42	103.38
31	у	1518	MA6	N1-C6-N6	6.21	123.59	117.06
33	2	55	PSU	N1-C2-N3	4.78	120.55	115.13
33	2	55	PSU	C4-N3-C2	-4.26	120.19	126.34
31	У	516	PSU	N1-C2-N3	4.23	119.93	115.13
31	У	1519	MA6	C3'-C2'-C1'	4.19	107.28	100.98
31	У	1519	MA6	N1-C6-N6	4.01	121.28	117.06
31	У	1518	MA6	C3'-C2'-C1'	3.94	106.91	100.98
31	У	516	PSU	C4-N3-C2	-3.75	120.94	126.34
33	2	55	PSU	C3'-C2'-C1'	3.45	105.65	101.64
31	У	1519	MA6	N3-C2-N1	-3.32	123.50	128.68
31	У	1207	2MG	CM2-N2-C2	-3.29	116.59	123.86
31	У	966	M2G	C3'-C2'-C1'	3.24	105.86	100.98
31	У	1404	5MC	C1'-N1-C6	-3.16	115.87	121.12
31	У	1404	5MC	C1'-N1-C2	3.13	125.41	118.42



Mol	Chain	$\mathbf{Res}$	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
31	У	967	5MC	CM5-C5-C6	-3.10	118.70	122.85
31	у	1518	MA6	N3-C2-N1	-2.95	124.06	128.68
31	у	516	PSU	C4'-O4'-C1'	-2.95	101.13	108.55
31	у	516	PSU	C6-N1-C2	-2.94	119.68	122.68
33	2	55	PSU	C6-N1-C2	-2.84	119.78	122.68
31	у	1519	MA6	C2'-C3'-C4'	2.82	108.11	102.64
31	у	527	7MG	C2-N3-C4	2.82	117.31	112.30
33	2	55	PSU	O2-C2-N1	-2.72	119.80	122.79
31	у	966	M2G	O3'-C3'-C2'	2.66	120.44	111.82
31	у	967	5MC	C3'-C2'-C1'	2.65	106.45	101.43
31	у	1518	MA6	O4'-C4'-C5'	2.63	118.04	109.37
31	у	1407	5MC	CM5-C5-C6	-2.56	119.44	122.85
31	у	527	7MG	N9-C4-N3	2.53	129.25	125.47
31	У	516	PSU	O2-C2-N1	-2.52	120.01	122.79
33	2	55	PSU	C6-C5-C4	2.51	119.95	118.20
31	у	1404	5MC	CM5-C5-C6	-2.50	119.51	122.85
31	у	527	7MG	C4-C5-N7	2.47	108.97	105.53
31	у	1404	5MC	C4'-O4'-C1'	-2.47	104.01	109.47
31	У	1207	2MG	O4'-C1'-C2'	-2.47	103.31	106.93
31	у	1407	5MC	C3'-C2'-C1'	2.34	105.87	101.43
31	у	527	7MG	C4'-O4'-C1'	-2.32	104.36	109.47
31	у	527	7MG	C5-C4-N3	-2.32	123.72	128.13
31	У	1407	5MC	C2'-C1'-N1	-2.26	106.82	113.22
31	у	1519	MA6	C10-N6-C9	2.23	123.31	116.12
31	У	1518	MA6	C1'-N9-C4	2.12	130.36	126.64
31	У	967	5MC	C1'-N1-C6	-2.12	117.60	121.12
31	у	1400	5MC	O3'-C3'-C4'	2.11	117.16	111.05
31	У	1518	MA6	O4'-C4'-C3'	2.06	109.19	105.11
31	У	1207	2MG	C8-N7-C5	2.04	106.87	102.99

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There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type	Atoms
31	У	1518	MA6	O4'-C4'-C5'-O5'
31	У	1518	MA6	C3'-C4'-C5'-O5'
31	У	1519	MA6	C5-C6-N6-C9
33	2	55	PSU	C2'-C1'-C5-C4
33	2	55	PSU	C2'-C1'-C5-C6
31	У	1404	5MC	C2'-C1'-N1-C2
31	У	1519	MA6	C5-C6-N6-C10
31	У	1404	5MC	C2'-C1'-N1-C6



Mol	Chain	Res	Type	Atoms
33	2	55	PSU	O4'-C1'-C5-C4
31	У	1519	MA6	N1-C6-N6-C9
31	У	1207	2MG	O4'-C4'-C5'-O5'
33	2	55	PSU	O4'-C1'-C5-C6

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There are no ring outliers.

No monomer is involved in short contacts.

#### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry (i)

There are no ligands in this entry.

#### 5.7 Other polymers (i)

There are no such residues in this entry.

#### 5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	W	35
31	У	9

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	W	41:C	O3'	43:G	Р	2.13
1	W	1506:C	O3'	1508:A	Р	2.09
1	W	489:G	O3'	491:G	Р	2.08
1	W	1448(B):A	O3'	1449:G	Р	2.07
1	W	436:C	O3'	438:G	Р	2.05
1	W	554:U	O3'	556:G	Р	2.05
1	W	1712:C	O3'	1716:U	Р	2.04
1	W	1743:G	O3'	1746:G	Р	2.04



Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	W	366(B):C	O3'	370:G	Р	2.03
1	W	890:A	O3'	892:G	Р	2.03
1	W	2213:U	O3'	2215:G	Р	2.03
1	W	2712(B):A	O3'	2713:A	Р	2.03
1	W	155:C	O3'	161:U	Р	2.02
1	W	926:A	O3'	928:G	Р	2.02
1	W	99:U	O3'	101:G	Р	2.01
1	W	1583:A	O3'	1585:C	Р	2.01
1	W	1718:G	O3'	1725:G	Р	2.01
1	W	1451:C	O3'	1453:A	Р	1.99
1	W	1481:U	O3'	1483:G	Р	1.99
1	W	1735:U	O3'	1741:C	Р	1.99
1	W	537:C	O3'	539:G	Р	1.98
1	W	1171:G	O3'	1173:G	Р	1.97
1	W	1864:U	O3'	1869:G	Р	1.97
1	W	1546(B):C	O3'	1547:C	Р	1.96
1	W	1630(B):C	O3'	1631:A	Р	1.96
1	W	1142(B):A	O3'	1143:A	Р	1.95
1	W	1872:A	O3'	1878:G	Р	1.95
1	W	2219:G	O3'	2224:G	Р	1.95
1	W	165:U	O3'	171:G	Р	1.94
1	W	1221(A):C	O3'	1222:C	Р	1.94
1	W	1444(B):A	O3'	1445:C	Р	1.93
1	W	1133:U	O3'	1135:C	Р	1.91
1	у	201:C	O3'	208:U	Р	1.89
1	W	2199:A	O3'	2205:C	Р	1.87
1	у	97:U	O3'	99:C	Р	1.83
1	W	2799:A	O3'	2801:A	Р	1.81
1	W	2795:G	O3'	2797:U	Р	1.79
1	у	99:C	O3'	101:A	Р	1.79
1	У	103(C):G	O3'	1033:G	Р	1.79
1	У	1455:G	O3'	1459:C	Р	1.78
1	У	843:U	O3'	848:C	Р	1.77
1	У	458:C	O3'	464:G	Р	1.76
1	У	102(C):C	O3'	1029:G	Р	1.76
1	у	136(B):C	O3'	1363:A	Р	1.76



# 6 Fit of model and data (i)

## 6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median,  $95^{th}$  percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ $>$	#RSRZ>2	$OWAB(Å^2)$	Q < 0.9
1	W	2889/2889~(100%)	0.03	107 (3%) 41 33	1,1,1,1	0
2	х	120/120~(100%)	-0.22	0 100 100	1,1,1,1	0
3	А	127/229~(55%)	-0.37	6 (4%) 31 26	1,1,1,1	0
4	В	272/276~(98%)	-0.14	19 (6%) 16 12	1,1,1,1	0
5	С	201/206~(97%)	-0.13	12 (5%) 21 17	1,1,1,1	0
6	D	194/205~(94%)	-0.64	0 100 100	1,1,1,1	0
7	Е	180/182~(98%)	-0.30	8 (4%) 34 29	1,1,1,1	0
8	F	173/180~(96%)	-0.46	8 (4%) 32 27	1,1,1,1	0
9	G	148/148~(100%)	-0.21	8 (5%) 25 21	1,1,1,1	0
10	Н	138/140~(98%)	-0.43	2 (1%) 75 67	1,1,1,1	0
11	Ι	122/122~(100%)	-0.17	8 (6%) 18 13	1,1,1,1	0
12	J	146/150~(97%)	-0.51	3 (2%) 63 55	1,1,1,1	0
13	Κ	137/141~(97%)	-0.08	11 (8%) 12 10	1,1,1,1	0
14	L	118/118~(100%)	-0.24	6 (5%) 28 24	1,1,1,1	0
15	М	106/112~(94%)	-0.16	5 (4%) 31 26	1, 1, 1, 1	0
16	Ν	137/146~(93%)	-0.24	3 (2%) 62 53	1,1,1,1	0
17	Ο	117/118~(99%)	-0.40	4 (3%) 45 37	1, 1, 1, 1	0
18	Р	101/101~(100%)	0.17	15 (14%) 2 2	1, 1, 1, 1	0
19	Q	109/113~(96%)	0.43	17 (15%) 2 2	1, 1, 1, 1	0
20	R	92/96~(95%)	-0.49	1 (1%) 80 74	1,1,1,1	0
21	S	103/110~(93%)	0.56	22 (21%) 0 1	1, 1, 1, 1	0
22	Т	185/206~(89%)	-0.41	5 (2%) 54 45	1, 1, 1, 1	0
23	U	76/85~(89%)	-0.41	1 (1%) 77 70	1, 1, 1, 1	0
24	V	88/98~(89%)	-0.30	2 (2%) 60 52	1, 1, 1, 1	0



Mol	Chain	Analysed	$<$ RSRZ $>$	#RSRZ>2	$OWAB(A^2)$	Q < 0.9
25	W	62/72~(86%)	-0.12	2 (3%) 47 38	1,1,1,1	0
26	Х	60/60~(100%)	-0.14	1 (1%) 70 62	1,1,1,1	0
27	Y	56/60~(93%)	-0.72	0 100 100	1,1,1,1	0
28	Z	48/49~(97%)	-0.69	0 100 100	1,1,1,1	0
29	a	63/65~(96%)	-0.07	5 (7%) 12 10	1,1,1,1	0
30	b	35/37~(94%)	0.97	11 (31%) 0 0	1,1,1,1	0
31	У	1504/1522~(98%)	0.04	62 (4%) 37 31	1,1,1,1	0
32	Z	77/77~(100%)	0.23	4 (5%) 27 23	1,1,1,1	0
33	2	75/76~(98%)	0.63	7 (9%) 8 7	1,1,1,1	0
34	3	18/18~(100%)	1.14	6 (33%) 0 0	1,1,1,1	0
35	с	234/256~(91%)	-0.28	10 (4%) 35 29	1,1,1,1	0
36	d	206/239~(86%)	-0.50	7 (3%) 45 37	1,1,1,1	0
37	е	208/209~(99%)	-0.40	6 (2%) 51 41	1,1,1,1	0
38	f	150/162~(92%)	-0.49	7 (4%) 31 26	1,1,1,1	0
39	g	101/101~(100%)	-0.56	2 (1%) 65 57	1,1,1,1	0
40	h	155/156~(99%)	-0.37	5 (3%) 47 38	1,1,1,1	0
41	i	138/138~(100%)	-0.04	11 (7%) 12 10	1,1,1,1	0
42	j	127/128~(99%)	-0.03	12 (9%) 8 7	1,1,1,1	0
43	k	98/105~(93%)	-0.32	2 (2%) 65 57	1,1,1,1	0
44	1	116/129~(89%)	0.07	12 (10%) 6 6	1,1,1,1	0
45	m	124/132~(93%)	-0.25	8 (6%) 18 14	1,1,1,1	0
46	n	125/126~(99%)	0.14	16 (12%) 3 4	1,1,1,1	0
47	О	60/61~(98%)	-0.50	2 (3%) 46 37	1,1,1,1	0
48	р	88/89~(98%)	0.18	11 (12%) 3 4	1,1,1,1	0
49	q	83/88~(94%)	1.02	21 (25%) 0 0	1,1,1,1	0
50	r	104/105~(99%)	-0.59	0 100 100	1,1,1,1	0
51	$\mathbf{S}$	81/88~(92%)	-0.65	0 100 100	1,1,1,1	0
52	t	80/93~(86%)	-0.11	6 (7%) 14 11	1, 1, 1, 1	0
53	u	99/106~(93%)	0.44	15 (15%) 2 2	1, 1, 1, 1	0
54	v	24/27~(88%)	-0.51	0 100 100	1, 1, 1, 1	0
All	All	10478/10865~(96%)	-0.11	524 (5%) 28 24	1, 1, 1, 1	0



Mol	Chain	Res	Type	RSRZ
34	3	7	G	9.1
31	у	145	G	8.0
41	i	52	ASP	7.4
1	W	2399	G	7.0
44	1	118	GLY	7.0
1	W	1067	А	6.7
1	W	1591	G	6.6
53	u	46	GLU	6.4
1	W	1473	G	6.4
46	n	124	PRO	6.4
41	i	57	PRO	6.3
31	у	144	G	6.2
1	W	1592	С	6.1
31	У	146	G	6.1
41	i	58	TYR	6.0
31	у	416	G	5.9
49	q	70	ALA	5.9
53	u	45	GLN	5.9
46	n	86	CYS	5.8
31	у	865	A	5.8
5	С	167	VAL	5.8
1	W	1983	С	5.7
21	S	34	LYS	5.7
1	W	2400	G	5.6
52	t	56	GLN	5.6
1	W	1679	U	5.6
1	W	1472	А	5.6
13	K	111	GLU	5.5
44	1	119	CYS	5.5
41	i	53	VAL	5.4
45	m	20	LYS	5.3
46	n	85	GLY	5.2
21	S	30	VAL	5.2
31	У	716	A	5.2
33	2	28	С	5.2
42	j	115	GLY	5.2
48	р	15	PHE	5.1
1	W	1116	С	5.1
38	f	13	ILE	5.1
42	j	123	PRO	5.0
41	i	54	ASP	5.0

All (524) RSRZ outliers are listed below:

HIS Continued on next page...

5.0

87

18

Р



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$\mathbf{Mol}$	Chain	$\operatorname{Res}$	Type	RSRZ
19	Q	85	VAL	5.0
4	В	109	ASP	5.0
42	j	116	LYS	5.0
22	Т	154	ASP	4.9
46	n	126	LYS	4.9
19	Q	97	LYS	4.9
30	b	13	LYS	4.8
19	Q	83	LYS	4.8
46	n	125	ARG	4.8
1	W	518	G	4.8
1	W	2398	U	4.8
52	t	57	HIS	4.7
33	2	34	G	4.7
30	b	29	ASN	4.7
25	W	19	VAL	4.7
48	р	16	ALA	4.7
31	y	23	C	4.7
19	Q	82	LEU	4.7
19	Q	95	ILE	4.7
1	W	1460	A	4.7
8	F	166	GLY	4.6
46	n	123	ALA	4.6
1	W	1635	G	4.6
44	1	115	PRO	4.5
46	n	83	ASP	4.5
21	S	5	MET	4.5
15	M	9	ARG	4.5
1	W	989	G	4.5
21	S	29	GLU	4.5
44	1	125	PHE	4.5
31	v	866	C	4.4
42	i	75	ASP	4.4
1	W	134	C	4.4
37	e	44	GLY	4.4
44	]	117	ASN	4.4
31	v	874	G	4.4
21	S	32	PRO	4.4
18	P	57	VAL	4.3
30	h	28	GLU	4.3
46	n	89	GLY	4.3
19	0	94	ASP	4.3
45	m v	19	LYS	4.3
10	111	1 10		1 1.0



Conti	Continued from previous page					
Mol	Chain	Res	Type	RSRZ		
44	1	126	ARG	4.3		
31	У	1079	G	4.2		
1	W	1405	U	4.2		
45	m	21	SER	4.2		
49	q	58	TYR	4.2		
41	i	51	VAL	4.2		
31	у	135	С	4.2		
37	е	46	LYS	4.2		
33	2	33	U	4.2		
18	Р	56	SER	4.2		
21	S	1	MET	4.2		
1	W	1221	С	4.1		
53	u	91	LEU	4.1		
48	р	3	ILE	4.1		
21	S	31	LEU	4.1		
4	В	198	ASN	4.1		
1	W	270(T)	G	4.1		
31	у	731	G	4.0		
5	Ċ	104	VAL	4.0		
4	В	199	ALA	4.0		
7	Е	49	ASP	4.0		
17	0	14	HIS	4.0		
30	b	8	LYS	4.0		
1	W	1590	U	4.0		
41	i	55	GLY	4.0		
1	W	2493	U	3.9		
22	Т	155	LEU	3.9		
31	y	1383	С	3.9		
31	y	227	G	3.9		
22	Ť	156	LYS	3.9		
30	b	12	ASP	3.9		
1	W	364	С	3.9		
9	G	16	GLY	3.9		
18	Р	86	GLY	3.9		
45	m	18	ARG	3.8		
34	3	6	G	3.8		
49	q	65	GLN	3.8		
14	L	59	ASP	3.8		
21	S	4	LYS	3.8		
1	W	1098	A	3.8		
19	Q	93	ALA	3.8		
38	f	14	ARG	3.8		



Mol	Chain	Res	Type	RSRZ
43	k	18	ALA	3.7
31	У	1535	С	3.7
18	Р	74	LYS	3.7
1	W	1680	U	3.7
19	Q	96	ILE	3.7
31	у	715	A	3.7
11	Ι	9	GLU	3.7
35	с	65	GLY	3.7
31	У	287	U	3.7
31	У	1078	U	3.7
5	С	5	LEU	3.7
1	W	2461	С	3.7
1	W	2600	A	3.7
41	i	56	LYS	3.6
1	W	1808	U	3.6
35	с	157	ARG	3.6
42	j	117	HIS	3.6
49	q	66	PRO	3.6
49	q	61	SER	3.6
31	У	1267	С	3.6
1	W	1764	G	3.6
1	W	1990	С	3.6
4	В	2	ALA	3.6
33	2	29	A	3.6
53	u	47	GLY	3.6
24	V	26	ARG	3.6
13	K	91	GLU	3.6
30	b	14	CYS	3.5
23	U	16	SER	3.5
1	W	1115	G	3.5
31	У	1117	G	3.5
49	q	21	VAL	3.5
1	W	2820	A	3.5
46	n	84	ILE	3.5
1	W	2492	U	3.5
21	S	92	ASN	3.5
34	3	8	U	3.5
32	Z	74	C	3.5
37	e	71	SER	3.5
13	K	110	THR	3.5
49	q	69	THR	3.5
18	Р	73	SER	3.5



Mol	Chain	Res	Type	RSRZ
46	n	79	LYS	3.5
46	n	72	ALA	3.4
13	K	32	PHE	3.4
11	Ι	69	VAL	3.4
13	K	131	ILE	3.4
49	q	24	ALA	3.4
31	У	611	А	3.4
1	W	2161	С	3.4
49	q	62	VAL	3.4
8	F	127	GLU	3.4
18	Р	88	ARG	3.4
30	b	7	VAL	3.3
29	a	19	SER	3.3
31	У	864	A	3.3
9	G	59	ALA	3.3
1	W	133	С	3.3
36	d	38	ARG	3.3
43	k	19	SER	3.3
1	W	2274	A	3.3
31	у	134	A	3.3
31	у	1342	С	3.3
11	Ι	70	LYS	3.3
42	j	105	ASP	3.3
31	у	677	U	3.3
1	W	1348	G	3.3
46	n	76	ALA	3.2
40	h	8	GLU	3.2
1	W	1600	С	3.2
1	W	1099	G	3.2
9	G	63	ALA	3.2
13	K	112	GLU	3.2
35	с	67	THR	3.2
3	А	39	ASP	3.2
4	В	110	GLY	3.2
1	W	270(V)	С	3.2
13	K	80	GLU	3.2
31	У	417	C	3.2
5	С	109	LYS	3.2
21	S	3	VAL	3.2
42	j	76	ALA	3.2
14	L	60	LEU	3.2
31	у	415	A	3.2



Mol	Chain	Res	Type	RSRZ
38	f	29	GLY	3.2
1	W	888	С	3.2
1	W	34	С	3.1
48	р	11	VAL	3.1
30	b	10	ILE	3.1
31	У	1536	С	3.1
35	с	37	ASN	3.1
49	q	36	ILE	3.1
9	G	60	GLU	3.1
49	q	19	ILE	3.1
13	К	92	GLY	3.1
44	1	121	PRO	3.1
1	W	241	А	3.1
8	F	165	ALA	3.1
1	W	1626	G	3.1
14	L	81	ASP	3.1
31	У	288	А	3.1
49	q	40	ASP	3.1
49	q	54	GLU	3.1
3	А	192	ALA	3.0
4	В	115	GLN	3.0
9	G	65	ALA	3.0
39	g	51	PRO	3.0
1	W	242	G	3.0
11	Ι	50	GLY	3.0
1	W	1026	U	3.0
4	В	96	HIS	3.0
42	j	13	ALA	3.0
37	е	95	GLY	3.0
48	р	4	THR	3.0
44	1	87	THR	3.0
21	S	27	VAL	3.0
21	S	26	LYS	3.0
38	f	15	ARG	3.0
48	р	80	ALA	3.0
1	W	270(U)	G	3.0
40	h	9	VAL	3.0
4	В	114	GLY	2.9
52	t	58	VAL	2.9
1	W	1369	G	2.9
38	f	12	LEU	2.9
31	у	179	А	2.9



Mol	Chain	Res	Type	RSRZ
31	У	1252	A	2.9
13	Κ	78	PRO	2.9
32	Z	17(A)	U	2.9
7	Е	126	ASP	2.9
1	W	1761	С	2.9
53	u	51	GLU	2.9
31	У	934	С	2.9
44	1	13	GLN	2.9
49	q	37	GLY	2.9
1	W	2145	С	2.9
1	W	2459	А	2.9
19	Q	21	VAL	2.9
4	В	65	ILE	2.9
31	у	861	G	2.9
5	С	168	MET	2.9
30	b	9	ARG	2.9
11	Ι	10	VAL	2.9
1	W	1989	G	2.9
31	у	714	G	2.9
33	2	65	G	2.9
12	J	93	GLY	2.8
45	m	49	SER	2.8
1	W	1349	A	2.8
1	W	1404	С	2.8
1	W	1068	G	2.8
49	q	59	TRP	2.8
13	K	79	LEU	2.8
1	W	23	G	2.8
30	b	27	CYS	2.8
31	У	262	A	2.8
34	3	18	С	2.8
8	F	129	THR	2.8
8	F	61	HIS	2.8
1	W	615	G	2.8
4	В	112	GLN	2.8
1	W	1498	С	2.8
29	a	27	THR	2.8
1	W	508	G	2.7
31	У	775	G	2.7
53	u	94	ALA	2.7
3	А	176	VAL	2.7
49	q	33	ILE	2.7



Mol	Chain	Res	Type	RSRZ
38	f	28	PHE	2.7
37	е	45	GLN	2.7
1	W	1678	G	2.7
25	W	18	PRO	2.7
37	е	29	PRO	2.7
8	F	56	SER	2.7
36	d	93	LYS	2.7
1	W	1625	С	2.7
17	0	17	ILE	2.7
29	a	6	THR	2.7
4	В	268	ARG	2.7
22	Т	153	SER	2.7
1	W	1474	С	2.7
42	j	72	GLY	2.7
42	j	114	TYR	2.7
1	W	2258	С	2.7
53	u	41	VAL	2.7
31	у	913	A	2.7
31	у	713	G	2.7
46	n	90	LEU	2.6
9	G	64	GLU	2.6
21	S	6	HIS	2.6
48	р	12	ILE	2.6
41	i	25	ASP	2.6
48	р	6	GLU	2.6
40	h	6	ARG	2.6
5	С	166	THR	2.6
7	Е	127	GLY	2.6
19	Q	101	SER	2.6
14	L	3	HIS	2.6
21	S	22	GLY	2.6
42	j	122	ALA	2.6
49	q	56	ALA	2.6
9	G	2	LYS	2.6
33	2	36	A	2.6
21	S	37	VAL	2.6
31	у	250	A	2.6
31	у	653	A	2.6
52	t	59	PRO	2.6
13	K	115	MET	2.5
9	G	67	ARG	2.5
21	S	25	GLY	2.5



Mol	Chain	Res	Type	RSRZ
31	У	1366	С	2.5
18	Р	76	LYS	2.5
1	W	2460	U	2.5
1	W	1301	A	2.5
4	В	200	ASP	2.5
26	Х	14	GLY	2.5
1	W	1977	А	2.5
3	А	177	GLY	2.5
7	Е	119	GLY	2.5
11	Ι	11	ALA	2.5
48	р	2	PRO	2.5
31	У	828	A	2.5
21	S	2	ARG	2.5
1	W	2599	G	2.5
45	m	27	LYS	2.5
1	W	1578	U	2.5
31	У	863	U	2.5
39	g	32	ASN	2.5
1	W	2248	С	2.5
35	с	66	GLY	2.5
1	W	2162	G	2.5
31	У	818	G	2.5
47	0	16	PHE	2.5
46	n	75	ALA	2.5
19	Q	84	ARG	2.5
1	W	85	G	2.5
1	W	680	G	2.5
35	с	231	GLU	2.5
18	Р	95	LEU	2.5
45	m	28	GLY	2.5
1	W	2260	С	2.5
8	F	168	PRO	2.5
49	q	22	THR	2.5
17	0	16	LYS	2.5
21	S	38	ILE	2.5
1	W	2012	G	2.4
4	В	126	GLN	2.4
36	d	189	ALA	2.4
1	W	1266	G	2.4
53	u	44	ALA	2.4
1	W	2730	С	2.4
3	А	195	ARG	2.4



Mol	Chain	Res	Type	RSRZ
18	Р	30	GLY	2.4
5	С	198	VAL	2.4
29	a	26	LYS	2.4
1	W	1807	G	2.4
41	i	50	ARG	2.4
1	W	1117	G	2.4
14	L	82	GLU	2.4
19	Q	13	SER	2.4
53	u	93	GLU	2.4
1	W	436	С	2.4
18	Р	29	PRO	2.4
1	W	1097	U	2.4
36	d	192	THR	2.4
21	S	35	TYR	2.4
40	h	94	ARG	2.4
52	t	65	ASN	2.4
3	А	196	ALA	2.4
44	1	114	VAL	2.4
1	W	1496	А	2.4
32	Z	17	С	2.4
16	N	66	VAL	2.3
35	с	158	LEU	2.3
47	0	11	LYS	2.3
44	1	12	ARG	2.3
4	В	3	VAL	2.3
5	С	110	GLY	2.3
21	S	90	LEU	2.3
31	У	241	С	2.3
18	Р	96	ILE	2.3
42	j	67	GLY	2.3
31	У	935	A	2.3
1	W	1577	С	2.3
49	q	20	VAL	2.3
1	W	1809	A	2.3
1	W	2345	G	2.3
1	W	1417	С	2.3
17	0	13	LYS	2.3
1	W	382	G	2.3
34	3	16	A	2.3
33	2	32	С	2.3
18	Р	72	VAL	2.3
1	W	1634	A	2.3


Mol	Chain	Res	Type	RSRZ
1	W	1636	С	2.3
19	Q	74	ALA	2.3
34	3	17	С	2.3
1	W	2076	U	2.3
48	р	9	GLN	2.3
53	u	90	GLN	2.3
1	W	256	А	2.3
32	Z	62	С	2.3
1	W	1593	G	2.3
7	Е	50	ALA	2.3
12	J	38	GLN	2.3
21	S	33	LYS	2.3
30	b	11	CYS	2.3
1	W	240	G	2.3
1	W	1692	U	2.3
22	Т	63	ASP	2.3
48	р	14	GLU	2.3
53	u	42	GLN	2.3
16	Ν	67	SER	2.3
20	R	65	ARG	2.3
1	W	1488	G	2.2
31	У	867	G	2.2
36	d	45	LYS	2.2
35	с	131	PRO	2.2
40	h	93	PRO	2.2
31	у	180	U	2.2
7	Е	165	THR	2.2
10	Н	42	GLU	2.2
19	Q	81	ALA	2.2
1	W	887	A	2.2
31	У	136	С	2.2
52	t	55	LYS	2.2
4	В	34	VAL	2.2
31	у	610	G	2.2
31	У	1187	G	2.2
5	С	197	ILE	2.2
31	У	78	G	2.2
36	d	41	GLY	2.2
1	W	1599	С	2.2
31	У	89	U	2.2
53	u	15	ARG	2.2
38	f	85	GLY 2.2	

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Mol	Chain	Res	Type	RSRZ
11	Ι	12	ASP	2.2
1	W	1368	G	2.2
1	W	2897	U	2.2
14	L	30	THR	2.1
31	У	676	А	2.1
31	У	79	G	2.1
31	У	1186	G	2.1
31	у	531	U	2.1
1	W	1665	А	2.1
10	Н	99	SER	2.1
18	Р	65	GLY	2.1
21	S	93	GLY	2.1
4	В	80	ALA	2.1
44	1	124	LYS	2.1
8	F	167	GLU	2.1
35	с	129	GLU	2.1
15	М	29	PHE	2.1
1	W	521	G	2.1
7	Е	47	LYS	2.1
46	n	36	LYS	2.1
46	n	122	LYS	2.1
19	Q	44	ALA	2.1
19	Q	86	LEU	2.1
4	В	45	ASN	2.1
4	В	108	PRO	2.1
53	u	49	ALA	2.1
36	d	39	ILE	2.1
31	у	88	С	2.1
45	m	26	LEU	2.1
49	q	1	MET	2.1
41	i	90	GLY	2.1
7	Ε	51	ARG	2.1
49	q	23	ASP	2.1
31	У	776	G	2.1
1	W	1095	A	2.1
1	W	2755	С	2.1
31	У	240	С	2.1
35	с	240	GLN	2.1
31	У	1166	G	2.1
19	Q	14	PRO 2.1	
31	У	136(A)	С	2.1
15	М	83	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
24	V	59	THR	2.0
4	В	95	LEU	2.0
5	С	199	ARG	2.0
53	u	48	LYS	2.0
1	W	1500	G	2.0
1	W	1666	G	2.0
1	W	1763	G	2.0
1	W	2731	G	2.0
5	С	114	ALA	2.0
15	М	37	ALA	2.0
16	N	70	VAL	2.0
12	J	37	GLY	2.0
18	Р	31	ALA	2.0
1	W	v 1633 C		2.0
5	С	196	VAL	2.0
1	W	820	A	2.0
53	u	9	ASN	2.0
15	М	28	VAL	2.0
29	a	5	LYS	2.0
11	Ι	13	ASN	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
33	PSU	2	55	20/21	0.82	0.24	1,1,1,1	0
31	M2G	У	966	25/26	0.92	0.14	1,1,1,1	0
31	PSU	У	516	20/21	0.92	0.17	1,1,1,1	0
31	5MC	У	1407	21/22	0.93	0.16	1,1,1,1	0
31	MA6	У	1518	24/25	0.93	0.17	1,1,1,1	0
31	MA6	У	1519	24/25	0.93	0.16	1,1,1,1	0
31	7MG	У	527	24/25	0.93	0.23	1,1,1,1	0
31	5MC	У	967	21/22	0.94	0.14	1,1,1,1	0
31	5MC	У	1404	21/22	0.94	0.20	1,1,1,1	0
31	2MG	У	1207	24/25	0.95	0.16	1,1,1,1	0
31	5MC	У	1400	21/22	0.97	0.24	1,1,1,1	0



## 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

## 6.4 Ligands (i)

There are no ligands in this entry.

## 6.5 Other polymers (i)

There are no such residues in this entry.

