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PDB ID	:	2WWB
EMDB ID	:	EMD-1652
Title	:	CRYO-EM STRUCTURE OF THE MAMMALIAN SEC61 COMPLEX
		BOUND TO THE ACTIVELY TRANSLATING WHEAT GERM 80S RI-
		BOSOME
Authors	:	Becker, T.; Mandon, E.; Bhushan, S.; Jarasch, A.; Armache, J.P.; Funes,
		S.; Jossinet, F.; Gumbart, J.; Mielke, T.; Berninghausen, O.; Schulten, K.;
		Westhof, E.; Gilmore, R.; Beckmann, R.
Deposited on	:	2009-10-22
Resolution	:	6.48 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/EMValidationReportHelp with specific help available everywhere you see the (i) symbol.

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

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

EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 6.48 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM} {f structures} \ (\#{f Entries})$
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for $\geq=3, 2, 1$ and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq=5\%$ The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length			Qu	ality of a	chain		
		1=0		34%					_
	А	476			:	88%			9% ••
			26	5%					
2	В	68				90%			9% •
			19%						
3	С	96		34%	••		63%		
			10%						
4	D	63	•	38%			51%		10%
	-		•						
5	E	34		539	%		44%	, D	•
			8%						
6	F	25			72%			28%	
7	G	14		36%			64%		



Mol	Chain	Length		Quality of cha	ain	
8	Н	362	48%	16%	9% •	26%
9	Ι	184	15%		19% 6	%• 17%
10	J	189	5% 26% ·		72%	
11	Κ	142	47%	9% •	42	2%
12	L	127	5%	74%		19% 6% •
13	М	113	58%		12% • •	26%
14	Ν	120	5%	9% ••	429	%
15	О	51	33%	31%	•••	27%



2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 14313 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

• Molecule 1 is a protein called PROTEIN TRANSPORT PROTEIN SEC61 SUBUNIT AL-PHA ISOFORM 1.

Mol	Chain	Residues		At	AltConf	Trace			
1	А	476	Total 3675	C 2409	N 591	O 650	$\begin{array}{c} \mathrm{S} \\ \mathrm{25} \end{array}$	0	0

• Molecule 2 is a protein called PROTEIN TRANSPORT PROTEIN SEC61 SUBUNIT GAMMA.

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace		
2	В	68	Total 543	C 355	N 94	O 89	${S \atop 5}$	0	0

• Molecule 3 is a protein called PROTEIN TRANSPORT PROTEIN SEC61 SUBUNIT BETA.

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace		
3	С	36	Total 281	C 188	N 44	0 47	${ m S} { m 2}$	0	0

• Molecule 4 is a RNA chain called 5.8S RRNA.

Mol	Chain	Residues		\mathbf{A}	AltConf	Trace			
4	D	63	Total 1347	C 603	N 245	0 436	Р 63	0	0

• Molecule 5 is a RNA chain called 25S RRNA.

Mol	Chain	Residues		\mathbf{A}^{\dagger}	toms	AltConf	Trace		
5	Е	34	Total 740	C 332	N 148	0 226	Р 34	0	0

• Molecule 6 is a RNA chain called 25S RRNA.

Mol	Chain	Residues		At	\mathbf{oms}	AltConf	Trace		
6	F	25	Total 536	C 239	N 99	0 173	Р 25	0	0



• Molecule 7 is a RNA chain called 25S RRNA.

Mol	Chain	Residues		Ate	oms	AltConf	Trace		
7	G	14	Total 296	C 133	N 54	O 96	Р 13	0	0

• Molecule 8 is a protein called 60S RIBOSOMAL PROTEIN L4-B.

Mol	Chain	Residues	Atoms			AltConf	Trace		
8	Н	269	Total 2039	C 1281	N 391	O 363	${S \atop 4}$	0	0

• Molecule 9 is a protein called 60S RIBOSOMAL PROTEIN L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace	
9	Ι	153	Total 1212	C 756	N 236	O 219	S 1	0	0

• Molecule 10 is a protein called 60S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues		Atc	\mathbf{ms}			AltConf	Trace
10	J	53	Total 410	C 254	N 83	0 72	S 1	0	0

• Molecule 11 is a protein called 60S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms				AltConf	Trace	
11	K	83	Total 663	C 424	N 111	O 126	${ m S} { m 2}$	0	0

• Molecule 12 is a protein called 60S RIBOSOMAL PROTEIN L26-A.

Mol	Chain	Residues	Atoms			AltConf	Trace		
12	L	127	Total 1002	C 630	N 193	0 178	S 1	0	0

• Molecule 13 is a protein called 60S RIBOSOMAL PROTEIN L31-A.

Mol	Chain	Residues	Atoms			AltConf	Trace		
13	М	84	Total 706	C 447	N 140	0 118	S 1	0	0

• Molecule 14 is a protein called 60S RIBOSOMAL PROTEIN L35.



Mol	Chain	Residues	Atoms				AltConf	Trace	
14	Ν	69	Total 547	C 345	N 101	O 99	${ m S} { m 2}$	0	0

 $\bullet\,$ Molecule 15 is a protein called 60S RIBOSOMAL PROTEIN L39.

Mol	Chain	Residues		Atc	\mathbf{ms}			AltConf	Trace
15	Ο	37	Total 316	C 200	N 66	0 48	$\frac{S}{2}$	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 atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: PROTEIN TRANSPORT PROTEIN SEC61 SUBUNIT ALPHA ISOFORM 1







WORLDWIDE PROTEIN DATA BANK





• Molecule 13: 60S RIBOSOMAL PROTEIN L31-A







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	221445	Depositor
Resolution determination method	Not provided	
CTF correction method	DEFOCUS GROUP VOLUMES	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	25	Depositor
Minimum defocus (nm)	1250	Depositor
Maximum defocus (nm)	4700	Depositor
Magnification	38000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	1.706	Depositor
Minimum map value	-0.671	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.100	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	455.4, 455.4, 455.4	wwPDB
Map dimensions	368, 368, 368	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	1.2375, 1.2375, 1.2375	Depositor



5 Model quality (i)

5.1 Standard geometry (i)

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	Bo	ond lengths	E	Bond angles
WIOI	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	1.89	8/3755~(0.2%)	1.10	22/5089~(0.4%)
2	В	0.94	0/553	1.12	2/738~(0.3%)
3	С	0.86	0/289	1.10	0/391
4	D	1.62	5/1508~(0.3%)	2.64	188/2348~(8.0%)
5	Е	1.67	2/833~(0.2%)	2.72	115/1298~(8.9%)
6	F	1.64	0/599	2.49	73/932~(7.8%)
7	G	1.70	2/330~(0.6%)	2.56	42/513~(8.2%)
8	Н	1.00	0/2079	1.46	33/2817~(1.2%)
9	Ι	1.03	0/1235	1.43	17/1662~(1.0%)
10	J	1.01	0/412	0.97	0/551
11	K	0.90	0/670	1.17	3/903~(0.3%)
12	L	1.02	0/1013	1.30	6/1351~(0.4%)
13	М	1.10	0/719	1.35	6/959~(0.6%)
14	N	1.05	1/549~(0.2%)	1.42	8/733~(1.1%)
15	0	1.10	0/321	1.45	4/426~(0.9%)
All	All	1.43	18/14865~(0.1%)	1.71	519/20711~(2.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	А	0	5
3	С	0	1
4	D	0	10
5	Е	0	6
6	F	0	3
7	G	0	1
8	Н	0	12
9	Ι	0	6
11	Κ	0	3
12	L	0	5



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Mol	Chain	#Chirality outliers	#Planarity outliers
13	М	0	2
14	Ν	0	2
15	0	0	7
All	All	0	63

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	104	ASP	N-CA	81.65	3.09	1.46
1	А	5	PHE	CG-CD2	29.16	1.82	1.38
1	А	5	PHE	CG-CD1	28.74	1.81	1.38
1	А	5	PHE	CE1-CZ	22.75	1.80	1.37
1	А	5	PHE	CE2-CZ	22.22	1.79	1.37
1	А	5	PHE	CD2-CE2	21.21	1.81	1.39
1	А	5	PHE	CD1-CE1	20.69	1.80	1.39
14	N	69	LEU	C-O	-12.08	1.00	1.23
4	D	53	А	N7-C5	-5.46	1.35	1.39
1	А	104	ASP	CA-CB	5.38	1.65	1.53
5	Е	544	А	N7-C5	-5.34	1.36	1.39
4	D	100	U	C2-N3	5.32	1.41	1.37
4	D	75	G	C2-N3	5.26	1.36	1.32
7	G	1928	G	N1-C2	5.21	1.42	1.37
4	D	103	G	C2-N3	5.13	1.36	1.32
7	G	1924	G	N1-C2	5.09	1.41	1.37
4	D	101	U	C2-N3	5.06	1.41	1.37
5	Е	548	G	N1-C2	5.04	1.41	1.37

All (519) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	Е	532	А	P-O3'-C3'	17.86	141.14	119.70
4	D	90	U	P-O3'-C3'	14.96	137.65	119.70
4	D	93	U	P-O3'-C3'	14.57	137.18	119.70
4	D	69	U	P-O3'-C3'	14.40	136.98	119.70
4	D	53	А	N1-C6-N6	14.32	127.19	118.60
4	D	65	А	P-O3'-C3'	13.29	135.65	119.70
4	D	96	A	P-O3'-C3'	13.27	135.62	119.70
5	Ε	557	A	N1-C6-N6	13.12	126.47	118.60
5	Е	530	A	N1-C6-N6	13.04	126.43	118.60
4	D	55	U	P-O3'-C3'	13.02	135.32	119.70
4	D	54	А	N1-C6-N6	12.98	126.39	118.60
5	Е	543	А	N1-C6-N6	12.94	126.37	118.60



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	Е	544	А	N1-C6-N6	12.91	126.35	118.60
6	F	1661	А	N1-C6-N6	12.83	126.30	118.60
4	D	41	А	N1-C6-N6	12.77	126.26	118.60
4	D	97	А	N1-C6-N6	12.73	126.24	118.60
5	Е	533	А	N1-C6-N6	12.66	126.19	118.60
5	Е	536	А	N1-C6-N6	12.58	126.15	118.60
6	F	1662	А	N1-C6-N6	12.50	126.10	118.60
4	D	52	А	N1-C6-N6	12.43	126.06	118.60
5	Е	555	А	N1-C6-N6	12.43	126.06	118.60
4	D	44	А	N1-C6-N6	12.41	126.04	118.60
4	D	88	А	N1-C6-N6	12.10	125.86	118.60
5	Е	549	А	N1-C6-N6	12.07	125.84	118.60
5	Е	554	А	N1-C6-N6	12.02	125.81	118.60
6	F	1667	А	N1-C6-N6	11.98	125.79	118.60
5	Е	531	А	N1-C6-N6	11.98	125.79	118.60
5	Е	545	А	N1-C6-N6	11.96	125.78	118.60
6	F	1673	А	N1-C6-N6	11.92	125.75	118.60
4	D	80	А	N1-C6-N6	11.92	125.75	118.60
4	D	65	А	N1-C6-N6	11.89	125.73	118.60
5	Е	556	А	N1-C6-N6	11.88	125.73	118.60
5	Е	535	А	N1-C6-N6	11.80	125.68	118.60
5	Е	553	А	N1-C6-N6	11.77	125.66	118.60
5	Е	560	А	N1-C6-N6	11.73	125.64	118.60
4	D	71	А	N1-C6-N6	11.64	125.58	118.60
4	D	72	А	N1-C6-N6	11.62	125.57	118.60
5	Е	542	А	N1-C6-N6	11.62	125.57	118.60
4	D	66	А	N1-C6-N6	11.60	125.56	118.60
7	G	1926	G	P-O3'-C3'	11.54	133.55	119.70
5	Ε	547	А	N1-C6-N6	11.52	125.51	118.60
4	D	61	А	N1-C6-N6	11.48	125.49	118.60
4	D	89	А	N1-C6-N6	11.40	125.44	118.60
4	D	96	А	N1-C6-N6	11.32	125.39	118.60
4	D	79	А	N1-C6-N6	11.31	125.39	118.60
7	G	1917	А	N1-C6-N6	11.22	125.33	118.60
4	D	43	А	N1-C6-N6	11.07	125.24	118.60
4	D	48	А	N1-C6-N6	11.02	125.21	118.60
6	F	1664	A	N1-C6-N6	11.00	125.20	118.60
7	G	1919	A	N1-C6-N6	10.98	125.19	118.60
6	F	1667	A	P-O3'-C3'	10.89	132.77	119.70
4	D	63	G	P-O3'-C3'	10.81	132.67	119.70
4	D	59	A	N1-C6-N6	10.69	125.02	118.60
4	D	92	А	N1-C6-N6	10.66	124.99	118.60



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	D	89	А	P-O3'-C3'	10.42	132.21	119.70
6	F	1678	G	N1-C6-O6	10.32	126.09	119.90
5	Е	560	А	P-O3'-C3'	10.31	132.08	119.70
4	D	63	G	N1-C6-O6	10.01	125.90	119.90
4	D	77	А	N1-C6-N6	9.95	124.57	118.60
6	F	1677	G	N1-C6-O6	9.93	125.86	119.90
6	F	1656	А	N1-C6-N6	9.88	124.53	118.60
1	А	104	ASP	N-CA-CB	9.83	128.30	110.60
6	F	1668	G	N1-C6-O6	9.82	125.80	119.90
7	G	1928	G	N1-C6-O6	9.80	125.78	119.90
7	G	1917	А	P-O3'-C3'	9.78	131.44	119.70
1	А	103	GLY	C-N-CA	9.68	145.91	121.70
5	Е	532	А	N1-C6-N6	9.59	124.35	118.60
7	G	1929	G	N1-C6-O6	9.58	125.65	119.90
5	Е	534	G	N1-C6-O6	9.57	125.64	119.90
5	Е	558	G	N1-C6-O6	9.54	125.62	119.90
5	Е	552	G	N1-C6-O6	9.40	125.54	119.90
4	D	56	G	N1-C6-O6	9.36	125.51	119.90
4	D	49	G	N1-C6-O6	9.34	125.50	119.90
5	Е	548	G	N1-C6-O6	9.33	125.50	119.90
7	G	1921	G	N1-C6-O6	9.25	125.45	119.90
4	D	58	G	N1-C6-O6	9.22	125.43	119.90
5	Е	546	G	N1-C6-O6	9.19	125.42	119.90
9	Ι	56	ARG	C-N-CA	9.18	144.64	121.70
4	D	103	G	N1-C6-O6	9.16	125.39	119.90
7	G	1922	U	O4'-C1'-N1	9.15	115.52	108.20
5	Ε	529	G	N1-C6-O6	9.15	125.39	119.90
6	F	1658	G	N1-C6-O6	9.14	125.38	119.90
6	F	1675	G	N1-C6-O6	9.12	125.38	119.90
6	F	1672	G	N1-C6-O6	9.07	125.34	119.90
5	Е	550	G	N1-C6-O6	9.06	125.34	119.90
4	D	78	G	N1-C6-O6	8.92	125.25	119.90
6	F	1665	G	N1-C6-O6	8.78	125.17	119.90
4	D	92	А	O4'-C1'-N9	8.74	115.19	108.20
4	D	42	G	N1-C6-O6	8.73	125.14	119.90
4	D	46	G	N1-C6-O6	8.72	125.13	119.90
4	D	87	G	N1-C6-O6	8.72	125.13	119.90
7	G	1926	G	N1-C6-O6	8.68	125.11	119.90
8	H	184	SER	C-N-CA	8.62	$143.2\overline{5}$	121.70
4	D	85	G	N1-C6-O6	8.57	125.05	119.90
5	Е	541	G	N1-C6-O6	8.57	125.05	119.90
4	D	63	G	C5-C6-O6	-8.55	123.47	128.60



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
6	F	1671	G	N1-C6-O6	8.54	125.02	119.90
9	Ι	56	ARG	CB-CA-C	8.48	127.35	110.40
4	D	68	G	N1-C6-O6	8.43	124.96	119.90
4	D	50	С	O4'-C1'-N1	8.39	114.91	108.20
6	F	1668	G	C5-C6-O6	-8.39	123.57	128.60
4	D	70	G	N1-C6-O6	8.34	124.90	119.90
5	Ε	558	G	C5-C6-O6	-8.34	123.60	128.60
4	D	102	U	O4'-C1'-N1	8.29	114.83	108.20
7	G	1924	G	N1-C6-O6	8.25	124.85	119.90
7	G	1925	С	O4'-C1'-N1	8.25	114.80	108.20
4	D	95	G	N1-C6-O6	8.23	124.84	119.90
4	D	62	С	O4'-C1'-N1	8.16	114.73	108.20
8	Н	54	GLU	C-N-CA	8.16	142.09	121.70
6	F	1670	U	O4'-C1'-N1	8.14	114.72	108.20
4	D	69	U	O4'-C1'-N1	8.09	114.67	108.20
8	Н	75	PRO	C-N-CA	8.07	141.88	121.70
6	F	1678	G	C5-C6-O6	-8.00	123.80	128.60
8	Н	59	GLN	C-N-CA	7.97	141.63	121.70
4	D	45	С	O4'-C1'-N1	7.91	114.52	108.20
11	Κ	123	TYR	CB-CG-CD1	-7.84	116.30	121.00
4	D	90	U	O4'-C1'-N1	7.80	114.44	108.20
7	G	1928	G	C5-C6-O6	-7.70	123.98	128.60
4	D	51	G	N1-C6-O6	7.67	124.50	119.90
4	D	81	U	O4'-C1'-N1	7.62	114.30	108.20
4	D	101	U	O4'-C1'-N1	7.62	114.29	108.20
8	Н	89	ALA	N-CA-CB	7.61	120.76	110.10
4	D	57	С	O4'-C1'-N1	7.59	114.27	108.20
1	А	104	ASP	CB-CA-C	-7.58	95.23	110.40
1	А	257	TYR	CB-CG-CD2	-7.58	116.45	121.00
5	Е	534	G	C5-C6-O6	-7.56	124.06	128.60
6	F	1657	С	O4'-C1'-N1	7.48	114.18	108.20
7	G	1927	С	O4'-C1'-N1	7.47	114.17	108.20
8	Н	60	THR	N-CA-CB	7.45	124.46	110.30
4	D	67	U	O4'-C1'-N1	7.45	114.16	108.20
6	F	1666	С	O4'-C1'-N1	7.42	114.13	108.20
5	Е	536	А	C5-C6-N6	-7.38	117.79	123.70
6	F	1677	G	C5-C6-O6	-7.37	124.18	128.60
9	Ι	36	ILE	C-N-CA	7.37	140.12	121.70
4	D	56	G	O4'-C1'-N9	7.34	114.07	108.20
6	F	1663	С	04'-C1'-N1	7.27	114.01	108.20
4	D	96	A	O4'-C1'-N9	7.26	114.01	108.20
5	Ε	540	U	O4'-C1'-N1	7.25	114.00	108.20



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
7	G	1923	С	O4'-C1'-N1	7.25	114.00	108.20
4	D	53	A	C5-C6-N6	-7.24	117.91	123.70
6	F	1672	G	C5-C6-O6	-7.24	124.26	128.60
5	Е	546	G	C5-C6-O6	-7.18	124.29	128.60
5	Е	548	G	C5-C6-O6	-7.18	124.29	128.60
11	К	123	TYR	CB-CG-CD2	7.17	125.30	121.00
5	Е	529	G	C5-C6-O6	-7.16	124.31	128.60
5	Е	530	А	C5-C6-N6	-7.14	117.99	123.70
5	Е	537	С	O4'-C1'-N1	7.14	113.91	108.20
4	D	76	С	N3-C4-N4	7.13	122.99	118.00
7	G	1924	G	C5-C6-O6	-7.12	124.33	128.60
4	D	85	G	C5-C6-O6	-7.12	124.33	128.60
5	Е	552	G	C5-C6-O6	-7.12	124.33	128.60
4	D	65	A	O4'-C1'-N9	7.11	113.89	108.20
7	G	1919	A	O4'-C1'-N9	7.10	113.88	108.20
4	D	99	С	O4'-C1'-N1	7.09	113.88	108.20
4	D	98	U	O4'-C1'-N1	7.08	113.87	108.20
4	D	53	А	C4-C5-C6	7.05	120.53	117.00
4	D	91	С	O4'-C1'-N1	7.04	113.83	108.20
13	М	25	PHE	CB-CG-CD2	7.04	125.72	120.80
4	D	103	G	C5-C6-O6	-7.03	124.38	128.60
4	D	46	G	C5-C6-O6	-7.03	124.38	128.60
4	D	47	С	O4'-C1'-N1	7.02	113.81	108.20
6	F	1654	С	O4'-C1'-N1	7.02	113.81	108.20
6	F	1658	G	C5-C6-O6	-7.01	124.40	128.60
4	D	49	G	C5-C6-O6	-7.00	124.40	128.60
6	F	1674	С	O4'-C1'-N1	7.00	113.80	108.20
4	D	55	U	O4'-C1'-N1	6.98	113.78	108.20
7	G	1929	G	O4'-C1'-N9	6.95	113.76	108.20
4	D	93	U	O4'-C1'-N1	6.94	113.75	108.20
6	F	1675	G	C5-C6-O6	-6.94	124.44	128.60
5	Е	544	A	C4-C5-C6	6.94	120.47	117.00
4	D	100	U	O4'-C1'-N1	6.94	113.75	108.20
4	D	68	G	C5-C6-O6	-6.92	124.44	128.60
4	D	78	G	C5-C6-O6	-6.90	124.46	128.60
7	G	1930	U	04'-C1'-N1	6.89	113.72	108.20
5	Е	539	U	O4'-C1'-N1	6.86	113.69	108.20
4	D	62	С	C6-N1-C1'	-6.86	112.57	120.80
4	D	62	C	C2-N1-C1'	6.85	126.34	118.80
9	Ι	71	ALA	N-CA-CB	6.84	119.67	110.10
4	D	91	C	N3-C4-C5	-6.84	119.17	121.90
4	D	64	U	O4'-C1'-N1	6.83	113.66	108.20



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
6	F	1659	U	O4'-C1'-N1	6.83	113.66	108.20
8	Н	75	PRO	CA-C-N	6.82	132.19	117.20
4	D	87	G	C5-C6-O6	-6.79	124.53	128.60
7	G	1929	G	C5-C6-O6	-6.78	124.53	128.60
1	А	5	PHE	CB-CG-CD1	-6.76	116.07	120.80
6	F	1671	G	C5-C6-O6	-6.75	124.55	128.60
12	L	84	LYS	C-N-CA	6.75	138.56	121.70
8	Н	72	ALA	N-CA-CB	6.74	119.54	110.10
7	G	1926	G	C5-C6-O6	-6.74	124.56	128.60
6	F	1656	А	O4'-C1'-N9	6.73	113.58	108.20
5	Е	528	U	O4'-C1'-N1	6.72	113.58	108.20
6	F	1661	А	C4-C5-C6	6.72	120.36	117.00
6	F	1655	С	O4'-C1'-N1	6.71	113.57	108.20
5	Е	541	G	O4'-C1'-N9	6.71	113.57	108.20
1	А	257	TYR	CB-CG-CD1	6.70	125.02	121.00
4	D	82	U	O4'-C1'-N1	6.70	113.56	108.20
5	Е	537	С	N3-C4-C5	-6.68	119.23	121.90
14	N	67	ARG	NE-CZ-NH2	6.68	123.64	120.30
5	Е	538	U	O4'-C1'-N1	6.67	113.54	108.20
4	D	58	G	C5-C6-O6	-6.67	124.60	128.60
8	Н	86	GLY	C-N-CA	6.66	138.36	121.70
13	М	25	PHE	CB-CG-CD1	-6.66	116.14	120.80
5	Е	551	U	O4'-C1'-N1	6.64	113.51	108.20
5	Е	548	G	O4'-C1'-N9	6.62	113.50	108.20
4	D	95	G	C5-C6-O6	-6.61	124.63	128.60
5	Е	550	G	C5-C6-O6	-6.59	124.64	128.60
7	G	1921	G	C5-C6-O6	-6.59	124.64	128.60
4	D	72	А	C4-C5-C6	6.59	120.30	117.00
5	Е	541	G	C5-C6-O6	-6.58	124.65	128.60
5	Ε	549	А	C4-C5-C6	6.58	120.29	117.00
6	F	1671	G	O4'-C1'-N9	6.57	113.46	108.20
6	F	1665	G	C5-C6-O6	-6.57	124.66	128.60
4	D	41	А	C5-C6-N6	-6.55	118.46	123.70
5	Ε	531	А	C5-C6-N1	-6.55	114.42	117.70
6	F	1675	G	O4'-C1'-N9	6.46	113.36	108.20
14	N	39	PRO	C-N-CA	6.45	137.82	121.70
5	E	543	A	C4-C5-C6	6.42	120.21	117.00
4	D	70	G	C5-C6-O6	-6.42	124.75	128.60
4	D	42	G	C5-C6-O6	-6.41	124.75	128.60
8	Н	87	GLN	N-CA-C	6.40	128.29	111.00
12	L	10	SER	C-N-CA	6.40	137.69	121.70
4	D	44	А	C5-C6-N6	-6.39	118.59	123.70



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Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^{o})$	$Ideal(^{o})$
4	D	43	А	O4'-C1'-N9	6.37	113.30	108.20
9	Ι	37	ASN	N-CA-CB	6.37	122.07	110.60
13	М	77	ARG	C-N-CA	6.37	137.61	121.70
6	F	1662	А	C5-C6-N6	-6.36	118.61	123.70
9	Ι	90	PHE	CB-CG-CD1	6.35	125.25	120.80
7	G	1926	G	O4'-C1'-N9	6.35	113.28	108.20
4	D	52	А	C4-C5-C6	6.35	120.18	117.00
4	D	52	А	C5-C6-N6	-6.35	118.62	123.70
4	D	83	С	C2-N1-C1'	6.34	125.77	118.80
4	D	76	С	O4'-C1'-N1	6.32	113.25	108.20
4	D	56	G	C5-C6-O6	-6.31	124.81	128.60
8	Н	84	ARG	N-CA-CB	6.29	121.92	110.60
4	D	72	А	C5-C6-N1	-6.28	114.56	117.70
5	Ε	542	А	C4-C5-C6	6.28	120.14	117.00
4	D	61	А	C5-C6-N1	-6.28	114.56	117.70
4	D	83	С	O4'-C1'-N1	6.27	113.21	108.20
6	F	1654	С	N3-C4-N4	6.25	122.37	118.00
6	F	1674	С	N3-C4-N4	6.24	122.37	118.00
5	Ε	553	А	C4-C5-C6	6.24	120.12	117.00
13	М	24	SER	N-CA-CB	6.23	119.85	110.50
8	Н	102	PRO	N-CA-C	6.22	128.28	112.10
4	D	73	U	O4'-C1'-N1	6.22	113.17	108.20
1	А	364	TYR	CB-CG-CD2	-6.22	117.27	121.00
9	Ι	39	TRP	N-CA-CB	6.21	121.78	110.60
4	D	92	А	C4-C5-C6	6.21	120.11	117.00
5	Е	533	А	C4-C5-C6	6.20	120.10	117.00
4	D	89	A	C4-C5-C6	6.20	120.10	117.00
8	Н	185	LYS	N-CA-C	6.18	127.69	111.00
8	Н	63	GLU	N-CA-C	-6.17	94.33	111.00
4	D	79	A	C4-C5-C6	6.17	120.08	117.00
5	E	557	A	C4-C5-C6	6.17	120.08	117.00
4	D	75	G	N1-C6-O6	6.17	123.60	119.90
7	G	1920	C	P-O3'-C3'	6.16	127.09	119.70
4	D	66	A	O4'-C1'-N9	6.15	113.12	108.20
4	D	88	A	C5-C6-N1	-6.15	114.62	117.70
5	Е	560	A	C4-C5-C6	6.14	120.07	117.00
5	Е	545	A	P-O3'-C3'	6.14	127.07	119.70
6	F	1667	A	C4-C5-C6	6.14	120.07	117.00
8	Н	214	GLY	C-N-CA	6.13	137.02	121.70
4	D	41	A	C4-C5-C6	6.11	120.06	117.00
5	Е	555	A	C4-C5-C6	6.11	120.06	117.00
5	Ε	533	А	C5-C6-N1	-6.11	114.65	117.70



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Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
4	D	42	G	O4'-C1'-N9	6.11	113.09	108.20
4	D	65	А	C4-C5-C6	6.10	120.05	117.00
4	D	89	А	O4'-C1'-N9	6.09	113.08	108.20
8	Н	58	HIS	N-CA-CB	6.09	121.57	110.60
4	D	54	А	C5-C6-N1	-6.08	114.66	117.70
9	Ι	56	ARG	CA-C-N	6.08	130.58	117.20
4	D	61	А	C4-C5-C6	6.08	120.04	117.00
5	Е	546	G	O4'-C1'-N9	6.08	113.06	108.20
6	F	1676	U	O4'-C1'-N1	6.07	113.06	108.20
4	D	50	С	N3-C4-C5	-6.07	119.47	121.90
5	Е	544	А	C5-C6-N6	-6.07	118.85	123.70
9	Ι	90	PHE	CB-CG-CD2	-6.07	116.55	120.80
5	Е	557	А	C5-C6-N1	-6.06	114.67	117.70
5	Е	557	А	C5-C6-N6	-6.06	118.85	123.70
6	F	1654	С	N3-C4-C5	-6.05	119.48	121.90
4	D	88	А	C4-C5-C6	6.05	120.03	117.00
5	Е	561	С	O4'-C1'-N1	6.05	113.04	108.20
1	А	104	ASP	N-CA-C	6.04	127.31	111.00
8	Н	55	LYS	N-CA-C	6.04	127.31	111.00
4	D	49	G	O4'-C1'-N9	6.03	113.03	108.20
4	D	57	С	N3-C4-N4	6.03	122.22	118.00
5	Е	556	А	C4-C5-C6	6.02	120.01	117.00
4	D	74	U	O4'-C1'-N1	6.02	113.02	108.20
5	Е	534	G	O4'-C1'-N9	6.02	113.01	108.20
5	Е	543	А	C5-C6-N1	-6.02	114.69	117.70
5	Е	547	А	C5-C6-N1	-6.02	114.69	117.70
6	F	1673	А	C5-C6-N6	-6.02	118.89	123.70
4	D	59	А	C4-C5-C6	6.01	120.01	117.00
4	D	54	А	O4'-C1'-N9	6.01	113.01	108.20
5	Ε	535	А	C4-C5-C6	6.01	120.00	117.00
9	Ι	105	LYS	C-N-CA	6.01	134.92	122.30
15	0	7	PHE	CB-CG-CD1	6.01	125.01	120.80
15	0	5	LYS	CB-CA-C	6.00	122.39	110.40
5	Ε	543	А	C5-C6-N6	-5.99	118.91	123.70
4	D	84	С	N3-C4-N4	5.99	122.19	118.00
5	Е	555	А	C5-C6-N6	-5.99	118.91	123.70
1	A	119	PHE	CB-CG-CD1	5.98	124.98	120.80
6	F	1655	C	N3-C4-C5	-5.97	119.51	121.90
5	E	529	G	O4'-C1'-N9	5.97	112.97	108.20
6	F	1661	A	C5-C6-N6	-5.96	118.93	123.70
8	H	159	ILE	C-N-CA	5.96	136.60	121.70
4	D	57	C	N3-C4-C5	-5.96	119.52	121.90



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	110	ALA	N-CA-CB	5.96	118.44	110.10
4	D	54	А	C5-C6-N6	-5.96	118.94	123.70
13	М	26	LYS	N-CA-CB	5.94	121.28	110.60
5	Е	532	А	O4'-C1'-N9	5.92	112.94	108.20
5	Е	560	А	O4'-C1'-N9	5.92	112.94	108.20
4	D	92	А	C5-C6-N1	-5.92	114.74	117.70
6	F	1658	G	O4'-C1'-N9	5.92	112.94	108.20
4	D	65	А	C5-C6-N1	-5.91	114.74	117.70
4	D	97	А	C5-C6-N1	-5.91	114.74	117.70
7	G	1920	С	N3-C4-C5	-5.90	119.54	121.90
6	F	1663	С	N3-C4-N4	5.90	122.13	118.00
4	D	80	А	O4'-C1'-N9	5.90	112.92	108.20
7	G	1924	G	O4'-C1'-N9	5.89	112.92	108.20
5	Е	547	А	C4-C5-C6	5.89	119.94	117.00
4	D	97	А	C5-C6-N6	-5.88	119.00	123.70
4	D	79	А	O4'-C1'-N9	5.87	112.90	108.20
6	F	1661	А	C5-C6-N1	-5.87	114.77	117.70
4	D	91	С	N3-C4-N4	5.85	122.09	118.00
7	G	1927	С	N3-C4-C5	-5.85	119.56	121.90
12	L	84	LYS	N-CA-CB	5.84	121.11	110.60
13	М	25	PHE	N-CA-CB	5.82	121.08	110.60
7	G	1917	А	C5-C6-N1	-5.82	114.79	117.70
4	D	63	G	O4'-C1'-N9	5.81	112.84	108.20
4	D	54	А	C4-C5-C6	5.80	119.90	117.00
5	Е	544	А	C5-C6-N1	-5.79	114.80	117.70
4	D	62	С	N3-C4-C5	-5.79	119.58	121.90
7	G	1918	С	O4'-C1'-N1	5.78	112.83	108.20
14	N	3	GLY	C-N-CA	5.78	136.15	121.70
6	F	1656	А	C5-C6-N1	-5.78	114.81	117.70
5	Е	554	А	C4-C5-C6	5.78	119.89	117.00
5	Е	545	А	C5-C6-N1	-5.77	114.82	117.70
5	Е	547	А	O4'-C1'-N9	5.76	112.81	108.20
4	D	47	С	N3-C4-N4	5.76	122.03	118.00
5	Е	530	А	C4-C5-C6	5.75	119.88	117.00
4	D	44	А	C4-C5-C6	5.75	119.88	117.00
5	Е	561	С	N3-C4-N4	5.75	122.02	118.00
9	Ι	105	LYS	CA-C-N	5.75	127.69	116.20
6	F	1668	G	O4'-C1'-N9	5.74	112.79	108.20
14	N	14	LYS	N-CA-CB	5.73	120.92	110.60
6	F	1674	С	N3-C4-C5	-5.73	119.61	121.90
4	D	45	С	N3-C4-N4	5.72	122.00	118.00
6	F	1667	А	C5-C6-N1	-5.72	114.84	117.70



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	D	86	U	O4'-C1'-N1	5.71	112.77	108.20
7	G	1925	С	N3-C4-N4	5.71	122.00	118.00
8	Н	88	GLY	C-N-CA	5.71	135.96	121.70
1	А	364	TYR	CB-CG-CD1	5.70	124.42	121.00
7	G	1925	С	N3-C4-C5	-5.70	119.62	121.90
4	D	80	А	C4-C5-C6	5.69	119.85	117.00
4	D	94	С	N3-C4-N4	5.68	121.98	118.00
7	G	1920	С	O4'-C1'-N1	5.68	112.75	108.20
5	Е	533	А	C5-C6-N6	-5.68	119.16	123.70
5	Е	542	А	C5-C6-N1	-5.68	114.86	117.70
5	Е	560	А	C5-C6-N1	-5.67	114.86	117.70
15	0	7	PHE	CB-CG-CD2	-5.67	116.83	120.80
1	А	119	PHE	CB-CG-CD2	-5.66	116.84	120.80
4	D	92	А	C5'-C4'-O4'	5.65	115.88	109.10
5	Е	554	А	C5-C6-N6	-5.64	119.18	123.70
4	D	53	А	C5-C6-N1	-5.64	114.88	117.70
5	Е	559	U	O4'-C1'-N1	5.64	112.71	108.20
8	Н	57	GLY	C-N-CA	5.63	135.78	121.70
7	G	1921	G	O4'-C1'-N9	5.63	112.70	108.20
4	D	70	G	O4'-C1'-N9	5.63	112.70	108.20
5	Е	549	А	C5-C6-N6	-5.63	119.20	123.70
4	D	59	А	C5-C6-N1	-5.62	114.89	117.70
5	Е	545	А	C4-C5-C6	5.61	119.81	117.00
4	D	71	А	C5-C6-N6	-5.61	119.21	123.70
5	Е	531	А	C4-C5-C6	5.61	119.80	117.00
4	D	51	G	C5-C6-O6	-5.60	125.24	128.60
4	D	99	С	N3-C4-N4	5.60	121.92	118.00
8	Н	54	GLU	N-CA-CB	5.59	120.67	110.60
8	Н	262	TRP	C-N-CA	5.58	134.03	122.30
12	L	125	LYS	N-CA-CB	5.58	120.65	110.60
15	0	31	THR	C-N-CA	5.58	135.66	121.70
4	D	43	А	C4-C5-C6	5.58	119.79	117.00
5	Е	561	С	N3-C4-C5	-5.58	119.67	121.90
5	Е	557	А	O4'-C1'-N9	5.57	112.66	108.20
4	D	75	G	C4-N9-C1'	5.57	133.74	126.50
14	N	13	SER	C-N-CA	5.55	135.59	121.70
4	D	59	A	O4'-C1'-N9	5.55	112.64	108.20
4	D	79	A	C5-C6-N1	-5.55	114.92	117.70
4	D	83	С	C6-N1-C1'	-5.55	114.14	120.80
7	G	1917	A	C4-C5-C6	5.55	119.77	117.00
7	G	1919	A	C4-C5-C6	5.55	119.78	117.00
6	F	1664	А	C5-C6-N1	-5.54	114.93	117.70



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	D	66	А	C4-C5-C6	5.54	119.77	117.00
6	F	1673	А	C4-C5-C6	5.54	119.77	117.00
4	D	94	С	N3-C4-C5	-5.54	119.68	121.90
6	F	1660	С	N3-C4-C5	-5.53	119.69	121.90
5	Е	549	А	C5-C6-N1	-5.53	114.94	117.70
5	Е	553	А	C5-C6-N1	-5.52	114.94	117.70
5	Е	556	А	C5-C6-N1	-5.52	114.94	117.70
4	D	80	А	C5-C6-N1	-5.52	114.94	117.70
6	\mathbf{F}	1666	С	N3-C4-N4	5.52	121.86	118.00
5	Ε	549	А	O4'-C1'-N9	5.50	112.60	108.20
6	F	1663	С	N3-C4-C5	-5.50	119.70	121.90
7	G	1923	С	N3-C4-N4	5.50	121.85	118.00
6	F	1660	С	O4'-C1'-N1	5.50	112.60	108.20
1	А	466	SER	N-CA-CB	5.49	118.74	110.50
4	D	80	А	C5-C6-N6	-5.49	119.31	123.70
9	Ι	3	ARG	C-N-CA	5.49	135.42	121.70
8	Н	77	VAL	CA-CB-CG1	5.48	119.12	110.90
5	Ε	535	А	C5-C6-N6	-5.47	119.32	123.70
8	Н	12	THR	C-N-CA	5.47	133.79	122.30
6	F	1655	С	N3-C4-N4	5.46	121.83	118.00
5	Ε	556	А	C5-C6-N6	-5.46	119.33	123.70
4	D	66	А	C5-C6-N1	-5.46	114.97	117.70
9	Ι	36	ILE	CA-C-N	5.45	129.19	117.20
4	D	75	G	C5-C6-O6	-5.45	125.33	128.60
9	Ι	57	ALA	N-CA-C	5.45	125.70	111.00
6	\mathbf{F}	1664	А	O4'-C1'-N9	5.44	112.55	108.20
1	А	324	TRP	N-CA-CB	5.44	120.39	110.60
14	Ν	39	PRO	CA-C-N	5.44	129.17	117.20
4	D	96	А	C4-C5-C6	5.44	119.72	117.00
4	D	96	А	C5-C6-N6	-5.43	119.36	123.70
6	F	1657	С	N3-C4-C5	-5.42	119.73	121.90
4	D	89	А	C5-C6-N6	-5.42	119.36	123.70
5	Ε	535	А	C5-C6-N1	-5.42	114.99	117.70
1	А	5	PHE	CB-CG-CD2	5.42	124.59	120.80
5	Ε	554	А	C5-C6-N1	-5.42	114.99	117.70
9	Ι	3	ARG	CB-CA-C	5.42	121.23	110.40
6	F	1667	A	C5-C6-N6	-5.42	119.37	123.70
5	E	553	A	C5-C6-N6	-5.41	119.38	123.70
4	D	75	G	N3-C2-N2	5.40	123.68	119.90
6	F	1666	С	N3-C4-C5	-5.39	119.74	121.90
6	F	1669	U	O4'-C1'-N1	5.39	112.51	108.20
5	Ε	545	А	C5-C6-N6	-5.39	119.39	123.70



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
7	G	1918	С	N3-C4-N4	5.39	121.77	118.00
14	N	37	SER	C-N-CA	5.39	135.17	121.70
1	А	141	SER	N-CA-CB	5.38	118.58	110.50
5	Е	542	А	O4'-C1'-N9	5.38	112.50	108.20
1	А	276	TYR	CB-CG-CD2	5.38	124.23	121.00
6	F	1664	А	C4-C5-C6	5.38	119.69	117.00
7	G	1928	G	O4'-C1'-N9	5.38	112.50	108.20
2	В	53	PHE	CB-CG-CD2	-5.37	117.04	120.80
4	D	77	А	C4-C5-C6	5.36	119.68	117.00
8	Н	28	ALA	N-CA-CB	5.36	117.61	110.10
5	Е	537	С	N3-C4-N4	5.35	121.75	118.00
8	Н	57	GLY	N-CA-C	-5.35	99.72	113.10
4	D	43	А	C5-C6-N1	-5.35	115.03	117.70
4	D	78	G	O4'-C1'-N9	5.34	112.48	108.20
4	D	99	С	N3-C4-C5	-5.34	119.76	121.90
5	Е	555	А	C5-C6-N1	-5.34	115.03	117.70
4	D	46	G	O4'-C1'-N9	5.34	112.47	108.20
4	D	47	С	N3-C4-C5	-5.33	119.77	121.90
4	D	66	А	C5-C6-N6	-5.32	119.44	123.70
7	G	1919	А	C5-C6-N1	-5.30	115.05	117.70
5	Е	553	А	O4'-C1'-N9	5.29	112.44	108.20
8	Н	105	THR	C-N-CA	5.29	134.93	121.70
14	Ν	69	LEU	CA-C-O	-5.29	108.99	120.10
4	D	85	G	O4'-C1'-N9	5.28	112.42	108.20
4	D	103	G	O4'-C1'-N9	5.26	112.41	108.20
5	Е	536	А	O4'-C1'-N9	5.26	112.41	108.20
4	D	65	А	C5-C6-N6	-5.26	119.49	123.70
4	D	71	А	C4-C5-C6	5.26	119.63	117.00
5	Е	560	А	C5-C6-N6	-5.25	119.50	123.70
4	D	88	А	C5-C6-N6	-5.25	119.50	123.70
7	G	1918	С	N3-C4-C5	-5.24	119.81	121.90
5	Е	532	А	C4-C5-C6	5.23	119.61	117.00
4	D	77	А	C5-C6-N1	-5.22	115.09	117.70
8	Н	100	PHE	CB-CG-CD1	5.22	124.45	120.80
4	D	58	G	04'-C1'-N9	5.22	112.38	108.20
4	D	77	А	O4'-C1'-N9	5.22	112.38	108.20
4	D	97	A	O4'-C1'-N9	5.22	112.37	108.20
6	F	1656	А	C4-C5-C6	5.21	119.61	117.00
9	Ι	9	THR	C-N-CA	5.19	134.67	121.70
4	D	44	A	O4'-C1'-N9	5.18	112.35	108.20
6	F	1662	А	O4'-C1'-N9	5.18	112.35	108.20
4	D	45	С	N3-C4-C5	-5.18	119.83	121.90



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	D	84	С	N3-C4-C5	-5.18	119.83	121.90
7	G	1927	С	N3-C4-N4	5.18	121.63	118.00
6	F	1660	С	N3-C4-N4	5.18	121.62	118.00
6	F	1677	G	O4'-C1'-N9	5.18	112.34	108.20
8	Н	12	THR	CA-C-N	5.17	126.55	116.20
5	Е	542	А	C5-C6-N6	-5.16	119.57	123.70
1	А	261	PHE	CB-CG-CD1	5.16	124.41	120.80
5	Е	531	А	O4'-C1'-N9	5.16	112.33	108.20
12	L	83	ASP	C-N-CA	5.16	134.59	121.70
4	D	51	G	N3-C2-N2	5.15	123.50	119.90
12	L	124	GLY	C-N-CA	5.15	134.57	121.70
8	Н	63	GLU	N-CA-CB	5.14	119.86	110.60
2	В	53	PHE	CB-CG-CD1	5.14	124.40	120.80
4	D	48	А	C5-C6-N6	-5.13	119.60	123.70
6	F	1678	G	O4'-C1'-N9	5.13	112.30	108.20
1	А	42	PHE	CB-CG-CD2	5.13	124.39	120.80
7	G	1928	G	P-O3'-C3'	5.12	125.84	119.70
5	Е	554	А	O4'-C1'-N9	5.09	112.27	108.20
5	Е	543	А	O4'-C1'-N9	5.09	112.27	108.20
7	G	1923	С	N3-C4-C5	-5.09	119.86	121.90
5	Е	550	G	O4'-C1'-N9	5.08	112.27	108.20
11	Κ	115	ARG	NE-CZ-NH1	5.08	122.84	120.30
8	Н	70	ALA	N-CA-C	-5.07	97.32	111.00
1	А	271	ARG	N-CA-CB	5.06	119.71	110.60
4	D	71	А	C5-C6-N1	-5.06	115.17	117.70
6	F	1654	С	C6-N1-C2	-5.05	118.28	120.30
4	D	53	А	O4'-C1'-N9	5.05	112.24	108.20
4	D	76	С	C5-C4-N4	-5.04	116.67	120.20
6	F	1657	С	N3-C4-N4	5.04	121.53	118.00
9	Ι	66	SER	C-N-CA	5.04	134.31	121.70
4	D	68	G	O4'-C1'-N9	5.04	112.23	108.20
4	D	73	U	C5'-C4'-C3'	-5.04	107.94	116.00
8	Н	86	GLY	N-CA-C	-5.04	100.51	113.10
5	Ε	535	А	O4'-C1'-N9	5.03	112.22	108.20
4	D	97	А	C4-C5-C6	5.03	119.52	117.00
1	А	276	TYR	CB-CG-CD1	-5.03	117.98	121.00
6	F	1672	G	O4'-C1'-N9	5.03	112.22	108.20
4	D	49	G	P-O5'-C5'	$5.0\overline{3}$	128.94	120.90
4	D	48	A	C5-C6-N1	-5.02	115.19	117.70
1	А	278	THR	N-CA-CB	5.02	119.84	110.30
4	D	79	A	C5-C6-N6	-5.02	119.69	123.70
4	D	89	А	C5-C6-N1	-5.02	115.19	117.70



Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
6	F	1664	А	C5-C6-N6	-5.02	119.69	123.70
8	Н	221	ASN	N-CA-CB	5.01	119.62	110.60
5	Ε	545	А	O4'-C1'-N9	5.01	112.21	108.20

There are no chirality outliers.

All (63) planarity outliers are listed below:

\mathbf{Mol}	Chain	Res	Type	Group
1	А	112	PHE	Sidechain
1	А	270	ALA	Peptide
1	А	271	ARG	Sidechain
1	А	336	TYR	Peptide
1	А	404	HIS	Sidechain
3	С	71	VAL	Peptide
4	D	46	G	Sidechain
4	D	50	С	Sidechain
4	D	55	U	Sidechain
4	D	56	G	Sidechain
4	D	62	С	Sidechain
4	D	65	A	Sidechain
4	D	66	А	Sidechain
4	D	76	С	Sidechain
4	D	77	А	Sidechain
4	D	87	G	Sidechain
5	Е	536	А	Sidechain
5	Е	541	G	Sidechain
5	Е	543	А	Sidechain
5	Е	545	А	Sidechain
5	Е	552	G	Sidechain
5	Е	558	G	Sidechain
6	F	1662	A	Sidechain
6	F	1667	А	Sidechain
6	F	1673	А	Sidechain
7	G	1925	С	Sidechain
8	Н	102	PRO	Peptide
8	Н	110	ASN	Peptide
8	Н	141	ARG	Sidechain
8	Н	148	ILE	Peptide
8	Н	187	LEU	Peptide
8	Н	197	ARG	Peptide
8	Н	209	TYR	Sidechain
8	Н	212	ASP	Peptide



Mol	Chain	Res	Type	Group
8	Н	63	GLU	Peptide
8	Н	73	ARG	Sidechain
8	Н	76	ARG	Peptide
8	Н	92	ASN	Peptide
9	Ι	122	ALA	Peptide
9	Ι	23	ARG	Sidechain
9	Ι	30	ARG	Sidechain
9	Ι	4	TYR	Sidechain
9	Ι	47	TYR	Sidechain
9	Ι	82	ARG	Sidechain
11	Κ	105	VAL	Peptide
11	Κ	57	LEU	Peptide
11	Κ	60	TYR	Sidechain
12	L	121	ARG	Peptide
12	L	125	LYS	Peptide
12	L	23	PRO	Peptide
12	L	40	ARG	Sidechain
12	L	52	ARG	Sidechain
13	М	10	ARG	Sidechain
13	М	74	ARG	Sidechain
14	N	32	LYS	Peptide
14	Ν	38	ARG	Sidechain
15	0	19	GLN	Peptide
15	0	23	LEU	Peptide
15	0	24	PRO	Peptide
15	0	30	ARG	Sidechain
15	0	32	ASN	Peptide
15	0	36	ARG	Peptide
15	0	4	GLN	Peptide

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5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	3675	0	3798	44	0
2	В	543	0	577	1	0
3	С	281	0	294	0	0
4	D	1347	0	678	2	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	Е	740	0	369	1	0
6	F	536	0	272	1	0
7	G	296	0	154	0	0
8	Н	2039	0	2106	16	0
9	Ι	1212	0	1231	8	0
10	J	410	0	452	0	0
11	K	663	0	699	4	0
12	L	1002	0	1093	2	0
13	М	706	0	741	1	0
14	N	547	0	613	8	0
15	0	316	0	349	2	0
All	All	14313	0	13426	81	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (81) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:5:PHE:CD2	1:A:5:PHE:CE2	1.81	1.68
1:A:5:PHE:CD1	1:A:5:PHE:CE1	1.80	1.66
1:A:5:PHE:CE2	1:A:5:PHE:CZ	1.79	1.64
1:A:5:PHE:CD1	1:A:5:PHE:CG	1.81	1.61
1:A:5:PHE:CE1	1:A:5:PHE:CZ	1.80	1.61
1:A:5:PHE:CD2	1:A:5:PHE:CG	1.82	1.59
1:A:5:PHE:CZ	1:A:104:ASP:HA	1.56	1.37
1:A:5:PHE:CE1	1:A:104:ASP:HA	1.82	1.14
1:A:5:PHE:CG	1:A:104:ASP:CA	2.39	1.05
1:A:5:PHE:CD2	1:A:104:ASP:CA	2.39	1.05
1:A:5:PHE:CE1	1:A:104:ASP:CA	2.41	1.03
1:A:5:PHE:CD1	1:A:104:ASP:CA	2.41	1.03
1:A:5:PHE:CE2	1:A:104:ASP:CA	2.42	1.01
1:A:5:PHE:CZ	1:A:104:ASP:CA	2.42	1.01
1:A:5:PHE:CD1	1:A:104:ASP:N	2.32	0.96
1:A:5:PHE:CD2	1:A:104:ASP:N	2.33	0.96
1:A:5:PHE:CG	1:A:104:ASP:N	2.33	0.95
1:A:5:PHE:CE2	1:A:104:ASP:N	2.35	0.94
1:A:5:PHE:CE1	1:A:104:ASP:N	2.37	0.93
1:A:5:PHE:CZ	1:A:104:ASP:N	2.39	0.90
1:A:5:PHE:CE2	1:A:104:ASP:HA	2.14	0.82
11:K:100:LYS:HA	11:K:105:VAL:HG22	1.67	0.76



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Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:5:PHE:CD1	1:A:104:ASP:C	2.62	0.73
1:A:5:PHE:CD2	1:A:104:ASP:CB	2.72	0.72
1:A:268:LYS:HB2	14:N:38:ARG:HH21	1.65	0.61
1:A:5:PHE:CE2	1:A:104:ASP:HB2	2.36	0.60
5:E:539:U:H3	5:E:546:G:H1	1.50	0.59
1:A:5:PHE:CE2	1:A:104:ASP:CB	2.86	0.58
9:I:57:ALA:HB3	9:I:82:ARG:O	2.06	0.56
1:A:277:ASN:H	14:N:38:ARG:HH22	1.56	0.55
12:L:56:VAL:HG22	12:L:106:ILE:HG22	1.88	0.54
1:A:94:LEU:HB3	1:A:112:PHE:CG	2.42	0.54
1:A:277:ASN:H	14:N:38:ARG:NH2	2.07	0.53
8:H:184:SER:HA	8:H:186:LYS:H	1.73	0.53
1:A:5:PHE:CD2	1:A:103:GLY:C	2.81	0.52
1:A:275:GLN:HB3	14:N:38:ARG:CZ	2.40	0.52
11:K:105:VAL:HG23	11:K:106:ASP:HA	1.91	0.52
8:H:88:GLY:HA3	8:H:89:ALA:HB3	1.92	0.52
8:H:58:HIS:CG	8:H:58:HIS:O	2.64	0.51
14:N:41:LEU:H	14:N:44:ILE:HD12	1.75	0.51
8:H:52:VAL:HG22	8:H:53:SER:H	1.76	0.50
8:H:198:ARG:CG	8:H:199:TRP:H	2.24	0.50
1:A:5:PHE:CD1	1:A:5:PHE:CB	2.84	0.50
2:B:20:ARG:HA	11:K:137:ASN:HD21	1.76	0.50
14:N:39:PRO:HB2	14:N:40:SER:C	2.32	0.49
9:I:3:ARG:HB2	9:I:4:TYR:HA	1.95	0.49
1:A:404:HIS:CE1	6:F:1657:C:H1'	2.48	0.49
8:H:184:SER:HA	8:H:186:LYS:N	2.28	0.49
8:H:57:GLY:HA3	8:H:58:HIS:HB2	1.95	0.48
1:A:268:LYS:CB	14:N:38:ARG:HH21	2.27	0.48
1:A:94:LEU:HB3	1:A:112:PHE:CD1	2.49	0.47
8:H:83:GLY:HA3	8:H:84:ARG:HB2	1.96	0.47
14:N:39:PRO:HA	14:N:41:LEU:HD22	1.96	0.47
9:I:9:THR:HG23	9:I:10:ASN:HA	1.98	0.46
1:A:273:ARG:HA	1:A:273:ARG:HE	1.81	0.46
9:I:108:ASP:HB2	9:I:109:ALA:HA	1.97	0.45
1:A:5:PHE:CD2	1:A:103:GLY:O	2.70	0.45
1:A:5:PHE:CD2	1:A:104:ASP:HB2	2.52	0.45
1:A:269:SER:HB2	1:A:403:GLY:H	1.82	0.45
8:H:63:GLU:CD	8:H:64:SER:H	2.20	0.45
8:H:152:VAL:HG12	8:H:153:SER:H	1.83	0.44
9:I:51:VAL:HG13	9:I:57:ALA:H	1.83	0.44
1:A:64:TRP:H	1:A:334:ARG:HE	1.65	0.44



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Atom 1	Atom 2	Interatomic	Clash			
Atom-1	Atom-2	distance (Å)	overlap (Å)			
1:A:271:ARG:HD3	1:A:272:TYR:CE2	2.53	0.44			
8:H:77:VAL:HG13	8:H:78:GLY:N	2.32	0.44			
8:H:222:VAL:HB	8:H:225:VAL:HG12	1.99	0.43			
8:H:74:ILE:H	8:H:75:PRO:HA	1.83	0.43			
11:K:105:VAL:HG23	11:K:106:ASP:CA	2.49	0.43			
1:A:108:ASP:HB2	1:A:112:PHE:CE1	2.55	0.42			
9:I:107:LEU:HD12	9:I:107:LEU:H	1.85	0.42			
9:I:24:VAL:HG11	9:I:87:SER:HA	2.02	0.42			
12:L:10:SER:N	12:L:11:ASP:HB2	2.35	0.42			
8:H:74:ILE:N	8:H:75:PRO:HA	2.35	0.41			
13:M:82:GLU:H	13:M:82:GLU:CD	2.22	0.41			
8:H:13:GLY:H	8:H:14:GLU:HB2	1.86	0.41			
4:D:55:U:C2	4:D:56:G:C8	3.08	0.41			
1:A:272:TYR:CE2	15:O:24:PRO:HG3	2.55	0.41			
1:A:5:PHE:CG	1:A:104:ASP:C	2.93	0.41			
9:I:138:LYS:H	9:I:138:LYS:HD3	1.86	0.41			
8:H:199:TRP:HA	8:H:200:THR:HB	2.02	0.41			
4:D:75:G:C2	15:O:27:ILE:HD13	2.56	0.40			

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	А	474/476~(100%)	402 (85%)	46 (10%)	26~(6%)	2 19
2	В	66/68~(97%)	60~(91%)	2(3%)	4~(6%)	1 17
3	С	34/96~(35%)	27~(79%)	4 (12%)	3~(9%)	1 11
8	Н	267/362~(74%)	181 (68%)	38 (14%)	48 (18%)	0 2
9	Ι	151/184~(82%)	119 (79%)	15 (10%)	17 (11%)	0 7
10	J	51/189~(27%)	46 (90%)	4 (8%)	1 (2%)	7 38



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Pe	erce	entiles
11	Κ	81/142~(57%)	73~(90%)	5~(6%)	3~(4%)		3	24
12	L	125/127~(98%)	101 (81%)	9~(7%)	15 (12%)		0	6
13	М	82/113~(73%)	65~(79%)	8 (10%)	9~(11%)		0	7
14	Ν	67/120~(56%)	59~(88%)	3~(4%)	5 (8%)		1	13
15	Ο	35/51~(69%)	26 (74%)	0	9~(26%)		0	1
All	All	1433/1928~(74%)	1159 (81%)	134 (9%)	140 (10%)		1	9

Continued from previous page...

All (140) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	56	SER
1	А	104	ASP
1	А	108	ASP
1	А	110	ALA
1	А	142	GLU
1	А	280	PRO
1	А	402	ARG
1	А	466	SER
1	А	473	ALA
2	В	30	ARG
2	В	41	ALA
3	С	71	VAL
3	С	72	PRO
8	Н	3	ARG
8	Н	28	ALA
8	Н	54	GLU
8	Н	55	LYS
8	Н	58	HIS
8	Н	60	THR
8	Н	63	GLU
8	Н	69	ARG
8	Н	70	ALA
8	Н	72	ALA
8	Н	74	ILE
8	Н	76	ARG
8	Н	87	GLN
8	Н	89	ALA
8	Н	98	ARG
8	Н	102	PRO
8	Н	103	THR



Mol	Chain	Res	Type
8	Н	146	PRO
8	Н	185	LYS
8	Н	187	LEU
8	Н	198	ARG
8	Н	199	TRP
8	Н	200	THR
8	Н	212	ASP
8	Н	222	VAL
8	Н	244	LEU
8	Н	262	TRP
9	Ι	37	ASN
9	Ι	57	ALA
9	Ι	67	ILE
9	Ι	107	LEU
9	Ι	111	LYS
9	Ι	113	TYR
9	Ι	123	PRO
9	Ι	143	PRO
12	L	23	PRO
12	L	85	VAL
12	L	125	LYS
13	М	78	LYS
13	М	79	ARG
13	М	90	PHE
14	Ν	4	VAL
14	N	14	LYS
14	Ν	39	PRO
15	0	20	ASN
15	0	22	PRO
15	Ο	23	LEU
1	A	107	LYS
1	А	141	SER
1	А	200	THR
1	A	226	LYS
1	А	324	TRP
2	В	66	VAL
8	H	13	GLY
8	Н	81	GLY
8	Н	93	MET
8	H	160	GLN
8	Н	173	GLY
8	Н	264	SER



Mol	Chain	Res	Type
9	Ι	7	THR
9	Ι	71	ALA
11	K	62	VAL
12	L	6	LEU
12	L	11	ASP
12	L	45	ILE
12	L	46	LYS
12	L	87	LYS
12	L	96	PRO
12	L	113	LYS
12	L	122	LYS
13	М	25	PHE
13	М	26	LYS
13	М	69	TYR
14	Ν	37	SER
15	0	5	LYS
15	0	6	SER
15	0	24	PRO
1	А	57	ASP
1	А	70	ALA
1	А	335	ALA
1	А	349	GLU
2	В	5	MET
8	Н	107	ARG
8	Н	132	ALA
8	Н	221	ASN
8	Н	265	GLU
9	Ι	2	ALA
9	Ι	3	ARG
9	Ι	25	SER
9	Ι	54	HIS
11	K	109	LYS
12	L	36	SER
12	L	84	LYS
14	N	5	LYS
15	0	25	GLN
1	А	105	THR
1	А	272	TYR
3	С	90	TRP
8	Н	101	ALA
8	Н	131	VAL
8	Н	215	ILE



Mol	Chain	Res	Type
9	Ι	39	TRP
11	K	131	ASP
12	L	97	ILE
13	М	24	SER
1	А	19	ILE
1	А	77	MET
1	А	443	SER
8	Н	52	VAL
8	Н	84	ARG
8	Н	106	TRP
8	Н	196	ASN
9	Ι	131	ARG
10	J	19	LYS
12	L	86	THR
15	0	34	THR
1	А	382	VAL
8	Н	4	PRO
8	Н	205	PRO
13	М	51	LEU
13	М	64	VAL
1	A	80	GLY
9	Ι	84	PRO
15	0	35	ILE
8	Н	86	GLY
1	A	8	VAL
8	H	77	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	398/398~(100%)	388~(98%)	10 (2%)	47	68
2	В	59/59~(100%)	57 (97%)	2(3%)	37	60
3	С	32/74~(43%)	32 (100%)	0	100	100
8	Н	209/288~(73%)	179 (86%)	30 (14%)	3	16



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
9	Ι	124/146~(85%)	107~(86%)	17 (14%)	3 17
10	J	44/154~(29%)	42 (96%)	2(4%)	27 52
11	Κ	74/118~(63%)	67~(90%)	7 (10%)	8 28
12	L	110/110~(100%)	95~(86%)	15 (14%)	3 17
13	М	74/97~(76%)	64 (86%)	10 (14%)	4 18
14	Ν	62/105~(59%)	57~(92%)	5 (8%)	11 35
15	Ο	33/46~(72%)	28~(85%)	5(15%)	3 15
All	All	1219/1595~(76%)	1116 (92%)	103 (8%)	14 34

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	5	PHE
1	А	25	LYS
1	А	68	ILE
1	А	232	GLU
1	А	263	VAL
1	А	327	THR
1	А	364	TYR
1	А	407	THR
1	А	414	ASN
1	А	465	GLN
2	В	5	MET
2	В	52	PHE
8	Н	4	PRO
8	Н	33	ASP
8	Н	35	VAL
8	Н	43	ASN
8	Н	46	LYS
8	Н	48	GLN
8	Н	77	VAL
8	Н	90	PHE
8	Н	98	ARG
8	Н	103	THR
8	Н	112	LYS
8	Н	119	ARG
8	Н	136	LEU
8	Н	140	HIS
8	Н	141	ARG
8	Н	145	ILE



Mol	Chain	Res	Type
8	Н	155	ASP
8	Н	159	ILE
8	Н	161	LYS
8	Н	162	THR
8	Н	164	GLU
8	Н	170	LYS
8	Н	193	LYS
8	Н	198	ARG
8	Н	201	GLN
8	Н	215	ILE
8	Н	233	LEU
8	Н	243	HIS
8	Н	244	LEU
8	Н	260	GLN
9	Ι	3	ARG
9	Ι	36	ILE
9	Ι	40	GLU
9	Ι	43	LYS
9	Ι	46	LYS
9	Ι	59	PRO
9	Ι	66	SER
9	Ι	67	ILE
9	Ι	72	GLN
9	Ι	76	PHE
9	Ι	79	THR
9	Ι	80	LYS
9	Ι	94	LEU
9	Ι	105	LYS
9	Ι	120	ASN
9	Ι	144	SER
9	Ι	149	VAL
10	J	1	MET
10	J	53	LYS
11	K	65	GLN
11	K	70	GLU
11	K	74	LYS
11	K	100	LYS
11	K	111	ASN
11	K	117	ASN
11	K	123	TYR
12	L	28	ARG
12	L	37	LYS



Mol	Chain	Res	Type
12	L	52	ARG
12	L	57	LEU
12	L	64	LYS
12	L	77	LYS
12	L	78	PHE
12	L	87	LYS
12	L	98	ASN
12	L	108	LYS
12	L	111	LEU
12	L	113	LYS
12	L	116	LYS
12	L	122	LYS
12	L	125	LYS
13	М	24	SER
13	М	38	LYS
13	М	47	ASP
13	М	62	ARG
13	М	67	VAL
13	М	77	ARG
13	М	79	ARG
13	М	82	GLU
13	М	86	LYS
13	М	92	TYR
14	N	5	LYS
14	N	9	LEU
14	N	34	GLN
14	N	38	ARG
14	N	39	PRO
15	0	17	LYS
15	0	18	LYS
15	0	22	PRO
15	0	23	LEU
15	0	26	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	277	ASN
2	В	58	HIS
8	Н	43	ASN
8	Н	213	ASN
11	К	111	ASN



Continued from previous page...

Mol	Chain	Res	Type
12	L	42	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	D	62/63~(98%)	27~(43%)	10 (16%)
5	Е	33/34~(97%)	9~(27%)	3~(9%)
6	F	24/25~(96%)	3 (12%)	0
7	G	14/14~(100%)	6 (42%)	2(14%)
All	All	133/136~(97%)	45 (33%)	15 (11%)

All (45) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	D	48	А
4	D	49	G
4	D	51	G
4	D	56	G
4	D	59	А
4	D	62	С
4	D	63	G
4	D	64	U
4	D	66	А
4	D	68	G
4	D	70	G
4	D	71	А
4	D	79	А
4	D	82	U
4	D	83	С
4	D	84	С
4	D	85	G
4	D	86	U
4	D	87	G
4	D	88	А
4	D	90	U
4	D	91	С
4	D	92	А
4	D	94	С
4	D	95	G
4	D	97	А
4	D	98	U



Mol	Chain	Res	Type
5	Е	532	А
5	Е	533	А
5	Е	534	G
5	Е	553	А
5	Е	556	А
5	Е	557	А
5	Е	558	G
5	Е	560	А
5	Е	561	С
6	F	1665	G
6	F	1666	С
6	F	1668	G
7	G	1918	С
7	G	1921	G
7	G	1922	U
7	G	1927	С
7	G	1929	G
7	G	1930	U

Continued from previous page...

All (15) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	D	48	А
4	D	51	G
4	D	55	U
4	D	63	G
4	D	65	А
4	D	69	U
4	D	89	А
4	D	90	U
4	D	93	U
4	D	96	А
5	Е	532	А
5	Е	558	G
5	Е	560	А
7	G	1917	А
7	G	1926	G

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

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



5.5 Carbohydrates (i)

There are no 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)

There are no chain breaks in this entry.



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-1652. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map



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

6.2 Central slices (i)

6.2.1 Primary map



X Index: 184



Y Index: 184



Z Index: 184



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

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 214

Y Index: 191

Z Index: 168

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



6.5 Mask visualisation (i)

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



7 Map analysis (i)

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

7.1 Map-value distribution (i)



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



7.2 Volume estimate (i)



The volume at the recommended contour level is 3348 nm^3 ; this corresponds to an approximate mass of 3024 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.



7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.154 \AA^{-1}



8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-1652 and PDB model 2WWB. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.



9.2 Q-score mapped to coordinate model (i)



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

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).



9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.



9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score	
All	0.6975	0.0920	
A	0.5775	0.0860	
В	0.6692	0.1140	1.0
С	0.3971	0.0410	
D	0.8189	0.0880	
Е	0.9351	0.1460	
F	0.8769	0.1340	
G	0.9426	0.1730	
Н	0.6628	0.0690	
Ι	0.6888	0.0790	
J	0.6667	0.1180	
К	0.6503	0.0970	0.0 0 .0
L	0.8564	0.0970	
М	0.7074	0.0760	
N	0.7425	0.0920	
0	0.5691	0.0980	

