



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 01:07 AM UTC

PDB ID : 3J45 / pdb_00003j45
EMDB ID : EMD-5692
Title : Structure of a non-translocating SecY protein channel with the 70S ribosome
Authors : Menetret, J.F.; Park, E.; Gumbart, J.C.; Ludtke, S.J.; Li, W.; Whynot, A.;
Rapoport, T.A.; Akey, C.W.
Deposited on : 2013-06-18
Resolution : 9.50 Å (reported)
Based on initial models : 2I2P, 3J01

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

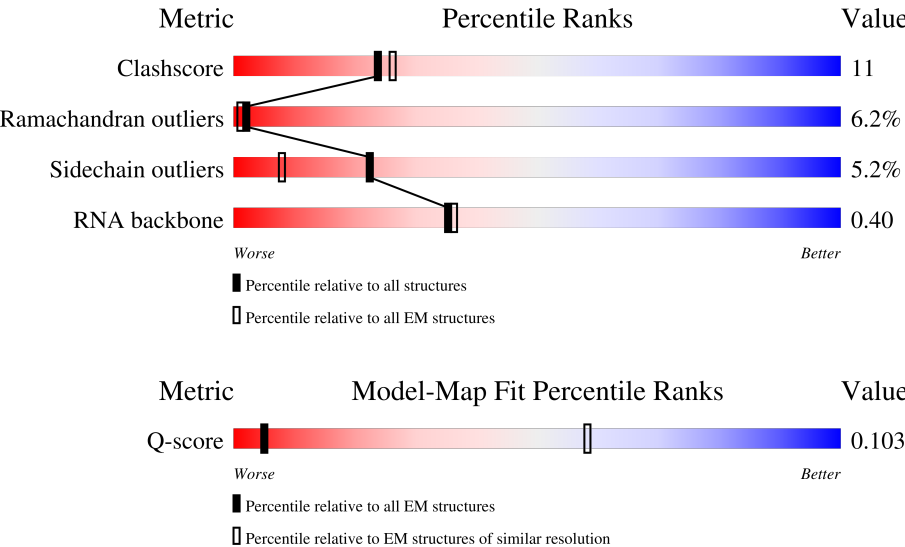
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance

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

The reported resolution of this entry is 9.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	234 (9.00 - 10.00)

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

Mol	Chain	Length	Quality of chain
1	y	437	16% 38% 50% 11% .
2	E	56	18% 39% 54% 7%
3	G	65	25% 40% 42% 15% .

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Mol	Chain	Length	Quality of chain
4	T	100	
5	U	103	
6	Y	63	
7	1	63	
8	2	36	
9	3	18	
10	4	61	
11	5	108	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 12465 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 translocase subunit SecY.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	y	437	Total	C	N	O	S	0	1
			3361	2220	554	570	17		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
y	5	ACE	-	acetylation	UNP P0AGA2
y	441	NH2	-	amidation	UNP P0AGA2

- Molecule 2 is a protein called Preprotein translocase subunit SecE.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	56	Total	C	N	O	S	0	1
			433	283	76	73	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	73	ACE	-	acetylation	UNP P0AG96
E	128	NH2	-	amidation	UNP P0AG96

- Molecule 3 is a protein called Protein-export membrane protein SecG.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	65	Total	C	N	O	S	0	0
			457	299	73	81	4		

- Molecule 4 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	T	100	Total	C	N	O	S	0	0
			787	496	146	143	2		

- Molecule 5 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	U	103	Total	C	N	O	0	0
			789	498	148	143		

- Molecule 6 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Y	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 7 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1	63	Total	C	N	O	P	0	0
			1350	603	245	439	63		

- Molecule 8 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	2	36	Total	C	N	O	P	0	0
			775	345	142	252	36		

- Molecule 9 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	3	18	Total	C	N	O	P	0	0
			387	172	71	126	18		

- Molecule 10 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	4	61	Total	C	N	O	P	0	0
			1312	584	240	427	61		

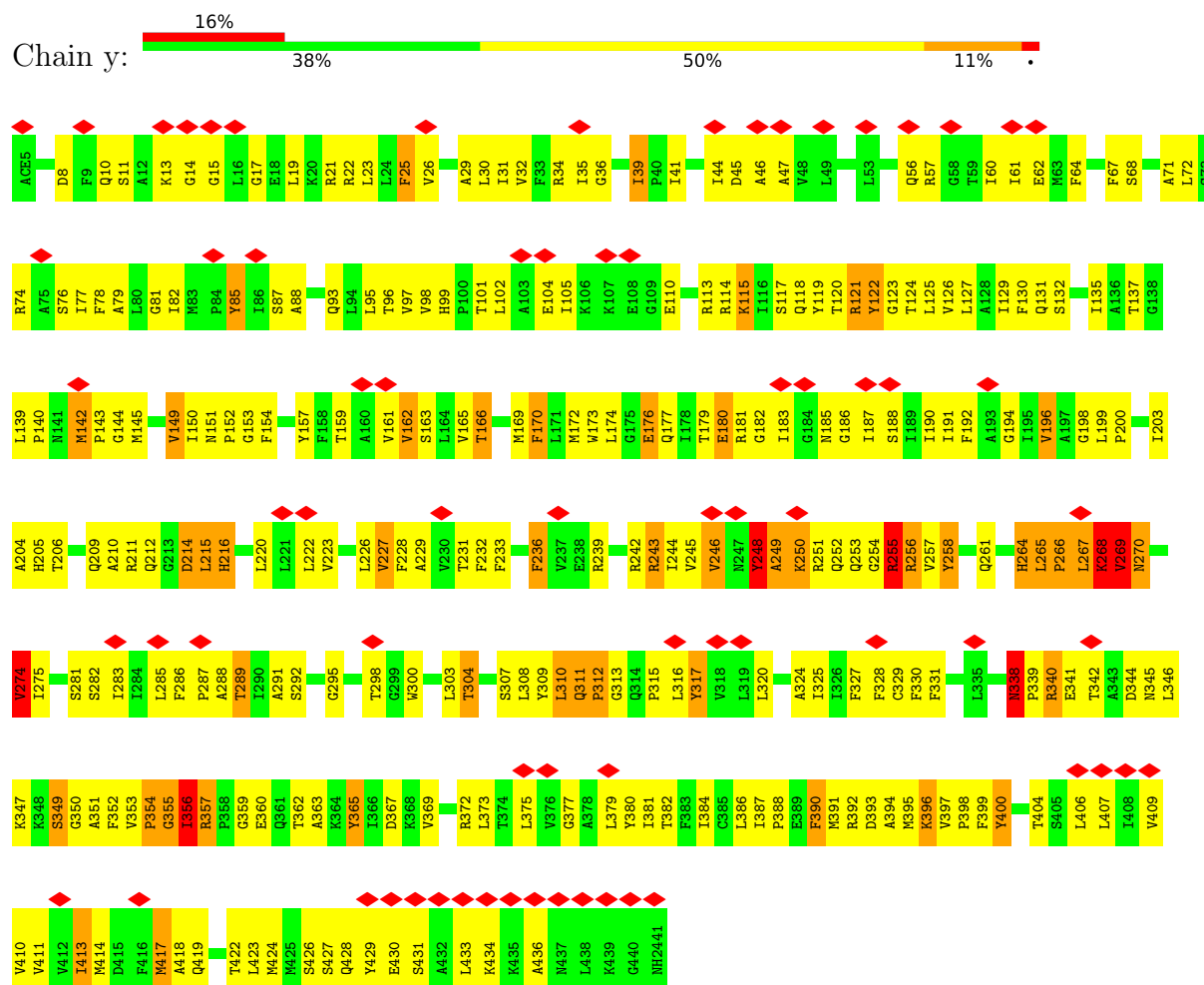
- Molecule 11 is a RNA chain called 23S ribosomal RNA.

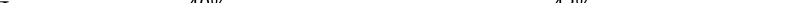
Mol	Chain	Residues	Atoms					AltConf	Trace
11	5	108	Total	C	N	O	P	0	0
			2305	1029	406	762	108		

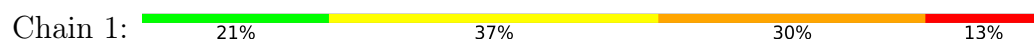
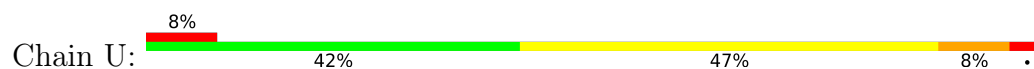
3 Residue-property plots

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 translocase subunit SecY



- Chain G:  25% 40% 42% 15%

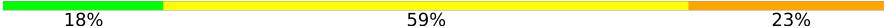


• Molecule 9: 23S ribosomal RNA

Chain 3:  44% 50% 6%

C1526	C1527	A1528	G1529	G1530	G1531	A1532	C1533	U1534	A1535	C1536	G1537	G1538	U1539	G1540	C1541	U1542	G1543
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• Molecule 10: 23S ribosomal RNA

Chain 4:  18% 59% 23%

C1838	G1839	G1840	U1841	G1842	C1843	C1844	G1845	G1846	A1847	A1848	G1849	G1850	U1851	A1852	A1853	A1854	U1855	U1856	G1857	A1858	U1859	G1860	G1861	G1862	G1863	U1864	U1865	A1866	G1867	C1868	G1869	C1870	A1871	A1872	G1873	G1874	G1875	A1876	A1877	G1878	C1879	U1880	C1881	U1882	U1883	G1884	A1885	U1886	C1887	G1888	A1889	G1890	G1891	C1892	C1893	G1894	C1895	G1896	G1897
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U1898

• Molecule 11: 23S ribosomal RNA

Chain 5:  8% 32% 44% 16%

U2092	C2093	C2094	A2095	C2096	A2097	U2098	U2099	U2100	A2101	C2102	C2103	G2104	U2105	G2106	G2107	A2108	U2109	G2110	U2111	G2112	U2113	A2114	G2115	G2116	A2117	U2118	A2119	G2120	G2121	U2122	G2123	G2124	G2125	A2126	G2127	G2128	C2129	U2130	U2131	U2132	G2133	A2134	A2135	G2136	U2137	G2138	U2139	G2140	G2141	A2142	C2143	G2144	C2145	G2146	A2147	G2148	U2149	C2150	U2151
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G2152	C2153	A2154	U2155	G2156	G2157	A2158	G2159	C2160	C2161	G2162	A2163	C2164	C2165	U2166	U2167	G2168	A2169	A2170	G2171	U2172	A2173	C2174	C2175	A2176	C2177	C2178	C2179	U2180	U2181	U2182	A2183	A2184	U2187	U2188	U2189	G2190	A2191	U2192	G2193	U2194	U2195	C2196	U2197	A2198	A2199
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	39000	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	per micrograph	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	51000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	11.232	Depositor
Minimum map value	-5.482	Depositor
Average map value	0.204	Depositor
Map value standard deviation	0.928	Depositor
Recommended contour level	1.8	Depositor
Map size ($\text{\AA}$)	393.12, 393.12, 393.12	wwPDB
Map dimensions	144, 144, 144	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	2.73, 2.73, 2.73	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NH2, ACE

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	y	2.29	130/3434 (3.8%)	2.55	263/4657 (5.6%)
2	E	2.30	12/437 (2.7%)	2.52	29/596 (4.9%)
3	G	0.30	0/462	1.88	15/620 (2.4%)
4	T	2.25	26/794 (3.3%)	2.32	38/1060 (3.6%)
5	U	2.30	32/797 (4.0%)	2.40	51/1062 (4.8%)
6	Y	2.40	25/510 (4.9%)	2.50	46/677 (6.8%)
7	1	2.02	28/1511 (1.9%)	1.75	41/2354 (1.7%)
8	2	1.99	13/867 (1.5%)	1.86	29/1351 (2.1%)
9	3	2.14	8/432 (1.9%)	1.71	11/672 (1.6%)
10	4	2.06	26/1468 (1.8%)	1.71	29/2289 (1.3%)
11	5	2.05	55/2577 (2.1%)	1.87	89/4015 (2.2%)
All	All	2.13	355/13289 (2.7%)	2.12	641/19353 (3.3%)

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	y	0	6
2	E	0	1
3	G	3	0
4	T	0	1
5	U	0	3
6	Y	0	1
7	1	0	30
8	2	0	15
9	3	0	10
10	4	0	20
11	5	0	54
All	All	3	141

All (355) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	T	73	ARG	CA-C	-15.02	1.42	1.52
1	y	139	LEU	C-N	12.81	1.43	1.33
2	E	124	GLY	CA-C	-9.47	1.41	1.52
5	U	42	LYS	CA-C	-9.44	1.41	1.52
1	y	176	GLU	N-CA	-9.24	1.34	1.46
7	1	77	G	C5'-C4'	8.97	1.64	1.51
1	y	229	ALA	CA-C	-8.69	1.41	1.52
1	y	331	PHE	C-N	8.58	1.44	1.33
1	y	239	ARG	NE-CZ	8.56	1.42	1.33
5	U	44	HIS	ND1-CE1	8.55	1.41	1.32
5	U	65	GLN	C-N	8.50	1.43	1.34
4	T	68	LYS	N-CA	-8.25	1.36	1.46
4	T	67	VAL	C-N	8.23	1.44	1.33
1	y	39	ILE	CA-C	-8.19	1.46	1.53
1	y	127	LEU	CA-C	-8.10	1.41	1.52
11	5	2190	G	C5'-C4'	8.08	1.63	1.51
1	y	10	GLN	CA-CB	8.03	1.65	1.53
4	T	3	ARG	NE-CZ	7.94	1.41	1.33
2	E	112	ASP	C-N	7.88	1.44	1.34
1	y	359	GLY	C-O	-7.78	1.20	1.24
1	y	78	PHE	CA-C	-7.75	1.42	1.52
4	T	77	ARG	NE-CZ	7.74	1.41	1.33
10	4	1844	C	P-O5'	-7.74	1.48	1.59
7	1	92	U	C5'-C4'	7.74	1.62	1.51
1	y	242	ARG	CD-NE	7.67	1.56	1.46
1	y	429	TYR	CA-C	-7.65	1.42	1.52
9	3	1539	U	C1'-N1	7.64	1.59	1.48
1	y	211	ARG	C-N	7.51	1.45	1.33
1	y	196	VAL	CA-CB	-7.48	1.45	1.54
1	y	216	HIS	CD2-NE2	7.48	1.46	1.37
4	T	26	LYS	CA-CB	7.47	1.65	1.53
11	5	2172	U	C2'-C1'	-7.44	1.41	1.53
6	Y	36	GLN	N-CA	-7.39	1.37	1.46
1	y	381	ILE	CA-CB	-7.35	1.46	1.54
1	y	357	ARG	CD-NE	7.32	1.56	1.46
5	U	3	LYS	CA-CB	7.29	1.64	1.54
2	E	79	VAL	N-CA	7.25	1.55	1.46
1	y	356	ILE	CA-C	-7.25	1.43	1.52
1	y	400	TYR	CA-C	-7.23	1.45	1.53
1	y	285	LEU	N-CA	-7.15	1.36	1.46
5	U	5	ARG	CD-NE	7.14	1.56	1.46
11	5	2184	A	C1'-N9	7.12	1.58	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	4	1847	A	C5'-C4'	7.07	1.61	1.51
1	y	31	ILE	CB-CG1	7.04	1.67	1.53
8	2	1323	C	C5'-C4'	7.03	1.61	1.51
1	y	150	ILE	CA-C	7.00	1.61	1.52
1	y	209	GLN	CA-C	-6.94	1.43	1.52
6	Y	30	MET	CA-C	-6.92	1.43	1.52
1	y	57	ARG	CA-C	-6.90	1.43	1.52
1	y	153	GLY	CA-C	-6.89	1.45	1.52
11	5	2188	U	O5'-C5'	6.87	1.52	1.42
4	T	26	LYS	N-CA	6.85	1.54	1.46
5	U	72	PHE	N-CA	-6.83	1.37	1.46
10	4	1843	C	C5'-C4'	6.82	1.61	1.51
7	1	85	G	P-O5'	-6.82	1.49	1.59
8	2	1314	C	O4'-C1'	6.81	1.51	1.41
6	Y	23	ARG	NE-CZ	6.80	1.40	1.33
11	5	2148	G	O3'-P	-6.79	1.50	1.61
1	y	431	SER	C-N	6.78	1.42	1.33
2	E	84	TRP	NE1-CE2	6.74	1.44	1.37
7	1	58	G	O3'-P	-6.72	1.51	1.61
7	1	85	G	C1'-N9	6.70	1.58	1.48
6	Y	52	ARG	CD-NE	6.65	1.55	1.46
5	U	85	ARG	NE-CZ	6.63	1.40	1.33
2	E	106	LEU	CA-C	-6.59	1.44	1.52
7	1	114	U	C1'-N1	6.57	1.58	1.48
6	Y	54	LYS	N-CA	-6.57	1.38	1.46
6	Y	7	ARG	NE-CZ	6.55	1.40	1.33
1	y	398	PRO	C-N	6.54	1.42	1.33
6	Y	13	GLU	CA-CB	6.54	1.63	1.53
4	T	34	VAL	CA-CB	-6.52	1.45	1.53
4	T	93	LEU	CA-C	-6.52	1.44	1.52
5	U	9	GLU	N-CA	-6.50	1.38	1.46
11	5	2141	G	C5'-C4'	6.49	1.60	1.51
1	y	365	TYR	C-N	6.49	1.41	1.33
1	y	388	PRO	N-CD	6.48	1.56	1.47
1	y	365	TYR	CA-CB	6.47	1.63	1.53
10	4	1854	A	C2'-C1'	-6.47	1.43	1.53
5	U	47	PRO	N-CA	-6.42	1.39	1.47
7	1	84	A	C4'-C3'	6.42	1.62	1.53
11	5	2146	C	C5'-C4'	6.42	1.60	1.51
11	5	2113	U	O4'-C1'	6.42	1.51	1.41
1	y	157	TYR	C-N	6.39	1.42	1.33
6	Y	23	ARG	C-N	6.38	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	y	214	ASP	N-CA	-6.38	1.38	1.46
11	5	2147	A	C2'-C1'	6.36	1.62	1.53
11	5	2144	G	C5'-C4'	6.36	1.60	1.51
1	y	181	ARG	CD-NE	6.35	1.55	1.46
6	Y	52	ARG	CZ-NH1	6.35	1.41	1.32
1	y	328	PHE	CA-CB	6.30	1.63	1.53
7	1	93	G	O4'-C1'	6.30	1.51	1.41
1	y	191	ILE	CA-C	-6.30	1.44	1.52
4	T	3	ARG	CZ-NH1	6.29	1.41	1.32
7	1	74	A	C2'-C1'	-6.26	1.43	1.53
5	U	12	VAL	C-N	6.25	1.42	1.33
1	y	436	ALA	C-N	6.24	1.42	1.33
10	4	1852	U	C5'-C4'	6.22	1.60	1.51
4	T	77	ARG	N-CA	-6.21	1.38	1.46
11	5	2130	U	O3'-P	-6.21	1.51	1.61
11	5	2132	U	C4'-O4'	6.21	1.55	1.45
2	E	91	LEU	CA-C	-6.21	1.45	1.52
7	1	64	A	O5'-C5'	6.21	1.51	1.42
10	4	1889	A	C4'-C3'	6.20	1.61	1.52
7	1	93	G	C3'-O3'	6.20	1.51	1.42
5	U	70	ALA	N-CA	-6.17	1.38	1.46
5	U	28	LEU	CA-CB	6.16	1.63	1.53
1	y	97	VAL	C-N	6.16	1.41	1.33
1	y	214	ASP	CA-C	-6.16	1.44	1.52
2	E	96	ILE	CA-C	-6.15	1.45	1.52
1	y	22	ARG	NE-CZ	6.15	1.39	1.33
8	2	1340	U	C3'-O3'	6.14	1.52	1.43
2	E	113	GLY	N-CA	6.13	1.54	1.45
1	y	216	HIS	CG-CD2	6.12	1.42	1.35
1	y	261	GLN	CA-CB	6.12	1.61	1.53
1	y	206	THR	C-N	6.11	1.41	1.33
9	3	1543	G	C5'-C4'	6.11	1.60	1.51
1	y	413	ILE	N-CA	-6.10	1.38	1.46
10	4	1852	U	C3'-C2'	-6.09	1.43	1.52
1	y	131	GLN	CA-CB	6.08	1.62	1.53
11	5	2153	C	C5'-C4'	6.08	1.60	1.51
1	y	257	VAL	C-N	6.07	1.42	1.33
5	U	24	VAL	CA-C	-6.05	1.47	1.53
4	T	1	MET	C-N	6.04	1.39	1.33
1	y	68	SER	C-N	6.02	1.42	1.33
8	2	1339	G	C5'-C4'	6.01	1.60	1.51
5	U	89	GLY	C-N	6.01	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	y	216	HIS	N-CA	-6.00	1.38	1.46
1	y	373	LEU	N-CA	-6.00	1.39	1.46
10	4	1859	U	C1'-N1	5.99	1.57	1.48
1	y	26	VAL	CA-C	5.98	1.59	1.52
1	y	288	ALA	N-CA	-5.98	1.39	1.46
1	y	369	VAL	C-N	5.98	1.41	1.33
11	5	2173	A	C5'-C4'	5.98	1.60	1.51
4	T	46	ALA	CA-C	-5.97	1.45	1.52
4	T	7	LEU	C-N	5.97	1.41	1.33
5	U	10	VAL	N-CA	-5.97	1.38	1.46
1	y	227	VAL	N-CA	-5.97	1.39	1.46
5	U	33	VAL	CA-C	-5.93	1.46	1.52
1	y	362	THR	CA-C	-5.93	1.45	1.52
1	y	433	LEU	CA-CB	5.92	1.63	1.53
5	U	87	GLU	N-CA	-5.92	1.39	1.46
11	5	2149	U	C5'-C4'	5.92	1.60	1.51
10	4	1858	A	C3'-O3'	5.92	1.51	1.42
1	y	289	THR	C-N	5.91	1.41	1.33
1	y	143	PRO	C-N	5.91	1.40	1.32
1	y	44	ILE	CA-C	-5.91	1.45	1.52
10	4	1896	G	C2'-C1'	-5.89	1.44	1.53
1	y	215	LEU	CA-C	-5.89	1.44	1.52
10	4	1850	G	C3'-O3'	5.87	1.50	1.42
11	5	2094	A	C3'-O3'	5.87	1.50	1.42
11	5	2160	C	C1'-N1	5.86	1.57	1.48
1	y	132	SER	CA-C	-5.86	1.44	1.52
7	1	89	A	C4'-C3'	5.85	1.61	1.52
11	5	2099	U	C2'-C1'	-5.85	1.44	1.53
1	y	227	VAL	CA-C	-5.84	1.45	1.52
11	5	2183	A	C4'-O4'	-5.84	1.36	1.45
1	y	232	PHE	CA-C	-5.84	1.45	1.52
11	5	2165	C	C1'-N1	5.83	1.57	1.48
9	3	1543	G	C4'-O4'	5.83	1.54	1.45
5	U	77	GLY	C-N	5.81	1.41	1.33
2	E	87	ARG	NE-CZ	5.80	1.39	1.33
5	U	9	GLU	CA-C	-5.80	1.45	1.52
1	y	257	VAL	CA-C	-5.79	1.45	1.52
7	1	112	U	C4'-C3'	5.79	1.61	1.52
1	y	78	PHE	CA-CB	5.78	1.63	1.53
7	1	60	G	C5'-C4'	5.78	1.60	1.51
1	y	199	LEU	CA-C	5.77	1.59	1.52
10	4	1890	A	O3'-P	5.77	1.69	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	5	2103	C	C4'-O4'	-5.76	1.36	1.45
1	y	210	ALA	CA-C	-5.74	1.45	1.52
7	1	91	A	C6-N6	5.74	1.45	1.33
1	y	281	SER	C-N	-5.74	1.26	1.33
7	1	114	U	C2-N3	5.73	1.49	1.37
6	Y	15	ASN	CA-C	5.72	1.60	1.52
5	U	21	ARG	CD-NE	5.72	1.54	1.46
10	4	1890	A	C1'-N9	5.72	1.56	1.48
6	Y	24	GLU	CA-CB	5.70	1.63	1.53
1	y	436	ALA	CA-C	5.69	1.60	1.52
11	5	2193	G	O5'-C5'	5.68	1.50	1.42
1	y	384	ILE	CA-C	5.68	1.59	1.52
1	y	231	THR	CA-C	-5.68	1.45	1.52
1	y	269	VAL	C-N	5.68	1.41	1.33
11	5	2104	C	C5'-C4'	5.68	1.59	1.51
11	5	2112	G	C1'-N9	5.67	1.56	1.48
1	y	382	THR	C-N	5.67	1.41	1.33
10	4	1856	U	C1'-N1	5.67	1.56	1.48
7	1	62	U	P-O5'	-5.67	1.51	1.59
8	2	1332	G	C2'-O2'	5.67	1.50	1.41
1	y	283	ILE	CA-CB	-5.66	1.47	1.54
10	4	1888	G	C1'-N9	5.66	1.56	1.48
1	y	250	LYS	N-CA	-5.66	1.38	1.46
1	y	95	LEU	C-N	5.64	1.41	1.33
11	5	2126	A	O5'-C5'	5.64	1.51	1.42
9	3	1529	G	C4'-C3'	-5.63	1.44	1.52
10	4	1876	A	O5'-C5'	5.62	1.50	1.42
11	5	2152	G	C3'-O3'	5.62	1.50	1.42
6	Y	27	ASN	CA-C	-5.62	1.45	1.52
11	5	2133	G	C4'-C3'	5.61	1.61	1.53
1	y	22	ARG	CA-C	-5.61	1.45	1.52
6	Y	40	SER	CA-C	-5.59	1.45	1.52
11	5	2137	U	C2'-C1'	5.59	1.61	1.53
1	y	220	LEU	C-N	5.58	1.41	1.33
6	Y	39	GLN	N-CA	-5.58	1.39	1.46
7	1	68	G	C3'-C2'	5.58	1.61	1.52
8	2	1317	G	O5'-C5'	5.57	1.50	1.42
10	4	1865	U	O3'-P	-5.56	1.52	1.61
6	Y	45	GLN	CA-C	-5.56	1.45	1.53
11	5	2098	U	N3-C4	5.56	1.49	1.38
4	T	39	THR	CA-C	-5.55	1.45	1.52
5	U	21	ARG	NE-CZ	5.54	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	y	74	ARG	CZ-NH2	5.54	1.40	1.33
1	y	121	ARG	CD-NE	5.54	1.53	1.46
1	y	17	GLY	C-N	5.53	1.41	1.33
1	y	304	THR	C-N	5.53	1.41	1.33
11	5	2122	U	P-O5'	-5.52	1.51	1.59
1	y	363	ALA	C-N	5.52	1.41	1.34
4	T	76	ARG	CD-NE	5.52	1.53	1.46
1	y	428	GLN	C-N	5.51	1.41	1.33
4	T	93	LEU	C-N	5.50	1.41	1.33
7	1	87	U	C1'-N1	5.49	1.56	1.48
6	Y	55	THR	CA-CB	-5.49	1.44	1.53
1	y	344	ASP	N-CA	5.48	1.52	1.46
11	5	2126	A	C4'-C3'	5.48	1.61	1.53
1	y	399	PHE	CA-CB	5.47	1.60	1.53
1	y	433	LEU	C-N	5.47	1.40	1.33
1	y	39	ILE	CA-CB	5.46	1.59	1.53
4	T	69	ARG	NE-CZ	5.46	1.39	1.33
10	4	1892	C	N1-C6	5.46	1.48	1.37
8	2	1325	U	C1'-N1	5.46	1.55	1.47
11	5	2174	C	C2'-O2'	-5.46	1.34	1.42
5	U	44	HIS	CA-C	-5.45	1.45	1.52
1	y	104	GLU	C-N	5.44	1.40	1.33
9	3	1539	U	C3'-C2'	5.43	1.60	1.52
1	y	99	HIS	CA-CB	5.41	1.60	1.53
11	5	2144	G	C4'-O4'	-5.41	1.37	1.45
8	2	1321	A	C3'-O3'	5.41	1.50	1.42
1	y	34	ARG	C-N	5.40	1.40	1.33
4	T	6	ARG	N-CA	-5.39	1.39	1.46
1	y	275	ILE	CA-CB	-5.39	1.51	1.54
7	1	63	A	C2'-C1'	-5.39	1.45	1.53
5	U	71	ILE	CA-CB	5.39	1.59	1.54
11	5	2096	C	P-O5'	-5.38	1.51	1.59
11	5	2175	C	C5'-C4'	5.38	1.59	1.51
11	5	2159	G	C5'-C4'	5.37	1.59	1.51
11	5	2191	A	O4'-C1'	5.37	1.49	1.41
1	y	19	LEU	C-N	5.36	1.40	1.33
5	U	27	VAL	CA-CB	5.36	1.61	1.54
10	4	1867	G	O3'-P	-5.36	1.53	1.61
1	y	392	ARG	CA-C	-5.36	1.45	1.52
1	y	67	PHE	C-O	-5.35	1.18	1.24
9	3	1539	U	C2'-C1'	-5.35	1.45	1.53
1	y	143	PRO	N-CA	-5.34	1.40	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	2	1316	U	C2'-C1'	-5.34	1.45	1.53
4	T	22	THR	N-CA	-5.34	1.39	1.46
7	1	56	A	C4'-C3'	5.33	1.60	1.52
5	U	64	ILE	C-N	5.32	1.40	1.33
11	5	2120	G	C2'-C1'	-5.32	1.45	1.53
7	1	52	A	C1'-N9	-5.32	1.40	1.48
10	4	1844	C	C3'-C2'	-5.31	1.44	1.52
1	y	182	GLY	CA-C	-5.31	1.44	1.51
11	5	2113	U	C2'-O2'	-5.30	1.34	1.42
11	5	2094	A	O3'-P	-5.29	1.53	1.61
5	U	5	ARG	CZ-NH1	5.29	1.40	1.32
11	5	2162	G	O3'-P	-5.28	1.53	1.61
4	T	23	ALA	C-N	5.28	1.39	1.33
1	y	424	MET	CA-C	-5.26	1.46	1.52
11	5	2153	C	C2'-C1'	-5.26	1.45	1.53
1	y	62	GLU	C-N	5.26	1.40	1.33
7	1	76	C	C2'-C1'	-5.25	1.45	1.53
6	Y	7	ARG	C-N	5.25	1.41	1.33
1	y	205	HIS	CE1-NE2	5.24	1.37	1.32
1	y	255	ARG	CZ-NH2	5.24	1.40	1.33
1	y	303	LEU	C-N	5.24	1.40	1.33
10	4	1860	G	C2'-C1'	-5.24	1.45	1.53
11	5	2199	A	C5'-C4'	5.24	1.59	1.51
10	4	1896	G	C5'-C4'	5.24	1.59	1.51
5	U	27	VAL	N-CA	-5.23	1.39	1.46
1	y	154	PHE	CA-CB	5.23	1.61	1.53
11	5	2119	A	C5'-C4'	5.23	1.59	1.51
1	y	315	PRO	CA-C	-5.22	1.47	1.52
7	1	64	A	C1'-N9	5.22	1.55	1.48
5	U	71	ILE	C-N	5.22	1.40	1.33
1	y	347	LYS	C-N	5.21	1.40	1.33
11	5	2123	G	C1'-N9	-5.21	1.40	1.48
1	y	82	ILE	N-CA	-5.21	1.39	1.46
1	y	96	THR	C-N	5.20	1.40	1.33
1	y	393	ASP	N-CA	-5.20	1.40	1.46
10	4	1860	G	P-O5'	5.20	1.67	1.59
1	y	391	MET	CA-C	-5.20	1.45	1.52
1	y	105	ILE	N-CA	-5.20	1.40	1.46
11	5	2132	U	C4'-C3'	5.20	1.60	1.53
11	5	2128	G	P-O5'	-5.19	1.51	1.59
6	Y	61	ALA	N-CA	-5.19	1.39	1.46
10	4	1891	G	O3'-P	5.19	1.69	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	5	2112	G	N9-C4	5.19	1.48	1.38
1	y	327	PHE	CA-CB	5.18	1.61	1.53
1	y	291	ALA	CA-C	-5.18	1.46	1.52
6	Y	29	ARG	CD-NE	5.17	1.53	1.46
7	1	72	U	C1'-N1	-5.17	1.39	1.47
4	T	69	ARG	CD-NE	5.16	1.53	1.46
5	U	69	VAL	CA-CB	-5.15	1.46	1.54
8	2	1326	U	C4'-O4'	-5.15	1.37	1.45
1	y	124	THR	CA-C	-5.14	1.46	1.52
1	y	190	ILE	CA-C	-5.14	1.45	1.52
1	y	434	LYS	CA-C	-5.14	1.46	1.52
4	T	86	THR	C-N	5.14	1.40	1.33
1	y	19	LEU	CA-C	-5.13	1.46	1.52
11	5	2104	C	P-O5'	5.13	1.67	1.59
1	y	426	SER	C-N	5.13	1.40	1.33
4	T	85	VAL	C-N	5.13	1.40	1.33
6	Y	28	LEU	CA-C	-5.13	1.46	1.52
1	y	222	LEU	CA-C	-5.12	1.46	1.52
7	1	75	G	C4'-C3'	5.12	1.60	1.52
7	1	90	U	O3'-P	-5.12	1.53	1.61
1	y	105	ILE	CB-CG1	5.12	1.63	1.53
8	2	1317	G	P-O5'	-5.12	1.52	1.59
1	y	249	ALA	CA-CB	-5.12	1.44	1.53
8	2	1313	U	C1'-N1	5.11	1.56	1.48
1	y	23	LEU	CA-CB	5.11	1.62	1.53
6	Y	22	LEU	CA-C	5.11	1.59	1.52
10	4	1893	C	C1'-N1	5.11	1.56	1.48
6	Y	48	ARG	CZ-NH1	5.10	1.39	1.32
6	Y	14	LEU	N-CA	5.10	1.52	1.46
9	3	1526	C	C4'-C3'	5.09	1.60	1.52
1	y	360	GLU	CA-C	-5.09	1.45	1.52
2	E	83	ILE	C-N	5.09	1.40	1.33
1	y	152	PRO	C-N	5.08	1.38	1.33
4	T	66	LYS	CA-CB	5.08	1.60	1.53
7	1	91	A	C3'-O3'	5.07	1.50	1.43
10	4	1868	C	C2'-C1'	-5.07	1.45	1.53
1	y	132	SER	C-N	5.07	1.40	1.33
8	2	1320	C	C1'-N1	5.07	1.55	1.47
5	U	81	ARG	NE-CZ	5.07	1.38	1.33
2	E	115	LEU	N-CA	5.07	1.52	1.46
11	5	2192	U	C5'-C4'	5.07	1.58	1.51
4	T	58	VAL	CA-CB	-5.06	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	y	212	GLN	C-N	5.05	1.38	1.32
11	5	2170	A	O4'-C1'	5.04	1.49	1.41
11	5	2138	G	C3'-O3'	5.04	1.49	1.42
6	Y	32	ALA	CA-C	-5.04	1.46	1.52
6	Y	21	LEU	C-O	-5.04	1.18	1.24
11	5	2170	A	O5'-C5'	-5.04	1.34	1.42
1	y	340	ARG	NE-CZ	5.04	1.38	1.33
11	5	2096	C	C2'-C1'	-5.03	1.45	1.53
11	5	2110	G	C5'-C4'	5.03	1.58	1.51
1	y	76	SER	CA-C	-5.03	1.46	1.52
9	3	1539	U	C3'-O3'	-5.03	1.34	1.42
1	y	145	MET	CA-C	-5.02	1.46	1.52
2	E	117	ARG	CZ-NH2	5.02	1.40	1.33
5	U	38	ILE	C-N	5.02	1.41	1.33
5	U	90	LYS	CA-CB	5.02	1.62	1.53
1	y	205	HIS	ND1-CE1	-5.01	1.27	1.32
1	y	95	LEU	CA-C	-5.00	1.45	1.52
1	y	105	ILE	CA-C	5.00	1.58	1.52
1	y	269	VAL	CA-CB	5.00	1.61	1.54

All (641) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	52	MET	N-CA-CB	18.30	141.41	110.49
3	G	51	PHE	N-CA-C	16.61	146.18	110.80
3	G	46	SER	N-CA-CB	-15.50	87.87	110.65
3	G	44	GLY	N-CA-C	13.59	145.39	113.18
1	y	268	LYS	N-CA-C	11.41	135.10	110.80
3	G	45	SER	N-CA-C	11.26	134.78	110.80
3	G	48	SER	CB-CA-C	11.08	132.47	110.42
1	y	269	VAL	N-CA-CB	11.01	129.40	111.23
2	E	117	ARG	N-CA-CB	10.98	125.99	110.07
6	Y	48	ARG	NE-CZ-NH2	10.83	128.95	119.20
2	E	80	ARG	NE-CZ-NH2	-10.64	109.62	119.20
1	y	149	VAL	N-CA-C	-10.46	100.50	111.58
8	2	1333	G	C4'-C3'-C2'	-10.22	92.38	102.60
11	5	2147	A	P-O3'-C3'	10.20	135.50	120.20
8	2	1315	C	P-O3'-C3'	10.11	135.37	120.20
5	U	89	GLY	N-CA-C	-9.60	101.74	115.27
3	G	50	ASN	N-CA-CB	-9.46	96.46	110.84
1	y	308	LEU	CA-C-N	9.17	132.57	120.28
1	y	308	LEU	C-N-CA	9.17	132.57	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	7	LEU	N-CA-C	-9.16	101.65	112.92
1	y	328	PHE	CA-CB-CG	-9.14	104.66	113.80
8	2	1333	G	P-O3'-C3'	9.08	133.82	120.20
1	y	29	ALA	CA-C-N	8.91	132.22	120.28
1	y	29	ALA	C-N-CA	8.91	132.22	120.28
1	y	341	GLU	CA-C-N	8.90	132.56	120.54
1	y	341	GLU	C-N-CA	8.90	132.56	120.54
5	U	50	ALA	N-CA-C	8.90	121.06	111.36
2	E	121	PHE	CA-C-N	8.87	135.54	120.29
2	E	121	PHE	C-N-CA	8.87	135.54	120.29
10	4	1870	C	C5'-C4'-C3'	-8.85	101.93	115.20
1	y	388	PRO	CA-C-N	8.79	131.87	120.44
1	y	388	PRO	C-N-CA	8.79	131.87	120.44
5	U	84	PHE	CA-CB-CG	-8.79	105.01	113.80
5	U	102	ILE	N-CA-C	-8.78	95.82	108.11
1	y	274	VAL	CA-C-N	8.77	128.85	120.43
1	y	274	VAL	C-N-CA	8.77	128.85	120.43
2	E	103	VAL	CA-C-N	8.77	132.03	120.28
2	E	103	VAL	C-N-CA	8.77	132.03	120.28
1	y	110	GLU	CA-C-N	8.68	131.91	120.28
1	y	110	GLU	C-N-CA	8.68	131.91	120.28
8	2	1311	G	O3'-P-O5'	-8.66	91.01	104.00
4	T	64	LYS	CB-CA-C	-8.66	100.33	111.50
11	5	2161	C	C4'-C3'-C2'	-8.63	93.97	102.60
1	y	367	ASP	CA-C-N	8.53	131.53	120.44
1	y	367	ASP	C-N-CA	8.53	131.53	120.44
1	y	347	LYS	CA-C-N	8.44	131.59	120.28
1	y	347	LYS	C-N-CA	8.44	131.59	120.28
4	T	2	ILE	N-CA-C	-8.38	104.61	111.81
1	y	113	ARG	CA-C-N	8.35	131.30	120.44
1	y	113	ARG	C-N-CA	8.35	131.30	120.44
3	G	46	SER	N-CA-C	-8.31	102.92	113.72
1	y	243	ARG	NE-CZ-NH2	-8.27	111.75	119.20
11	5	2137	U	O4'-C1'-N1	8.27	120.91	108.50
11	5	2148	G	P-O3'-C3'	8.27	132.60	120.20
1	y	187	ILE	N-CA-CB	8.24	120.19	110.55
4	T	92	ASN	N-CA-C	-8.16	97.00	109.41
1	y	26	VAL	N-CA-CB	8.12	119.47	110.62
1	y	95	LEU	N-CA-CB	7.99	123.42	110.40
1	y	205	HIS	O-C-N	7.98	130.29	122.07
5	U	45	GLN	OE1-CD-NE2	-7.97	114.62	122.60
1	y	88	ALA	N-CA-C	7.96	119.96	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	35	ALA	N-CA-C	7.93	119.56	111.07
4	T	22	THR	N-CA-C	-7.91	103.47	113.43
1	y	255	ARG	N-CA-CB	7.87	123.79	110.49
1	y	380	TYR	CA-C-N	7.86	130.74	120.60
1	y	380	TYR	C-N-CA	7.86	130.74	120.60
1	y	139	LEU	O-C-N	-7.73	113.60	120.48
1	y	414	MET	N-CA-CB	7.71	121.75	110.26
1	y	99	HIS	CA-C-O	-7.67	113.06	120.19
11	5	2153	C	C5'-C4'-C3'	-7.66	103.71	115.20
8	2	1336	A	P-O5'-C5'	7.63	132.35	120.90
1	y	129	ILE	CA-C-N	7.61	130.48	120.28
1	y	129	ILE	C-N-CA	7.61	130.48	120.28
4	T	43	ILE	N-CA-C	-7.60	101.63	112.35
11	5	2116	G	C4'-C3'-C2'	7.60	110.20	102.60
1	y	204	ALA	CA-C-N	7.59	130.31	120.44
1	y	204	ALA	C-N-CA	7.59	130.31	120.44
1	y	404	THR	CA-C-N	7.59	130.45	120.28
1	y	404	THR	C-N-CA	7.59	130.45	120.28
4	T	72	GLN	CA-C-N	7.59	130.75	121.64
4	T	72	GLN	C-N-CA	7.59	130.75	121.64
1	y	115	LYS	N-CA-C	7.53	119.49	111.28
1	y	36	GLY	CA-C-N	7.52	130.35	120.28
1	y	36	GLY	C-N-CA	7.52	130.35	120.28
1	y	186	GLY	CA-C-N	7.49	130.00	120.56
1	y	186	GLY	C-N-CA	7.49	130.00	120.56
11	5	2161	C	P-O3'-C3'	7.42	131.34	120.20
1	y	97	VAL	CA-C-O	-7.42	113.23	120.95
1	y	161	VAL	CA-C-N	7.39	129.87	120.56
1	y	161	VAL	C-N-CA	7.39	129.87	120.56
11	5	2119	A	O4'-C1'-N9	7.38	119.28	108.20
5	U	100	GLU	CB-CG-CD	-7.38	100.05	112.60
5	U	46	LYS	N-CA-C	7.37	120.09	109.48
1	y	282	SER	N-CA-CB	7.36	120.68	110.01
7	1	68	G	C4'-C3'-C2'	-7.36	95.24	102.60
5	U	68	ASN	N-CA-C	-7.35	102.92	113.21
11	5	2120	G	P-O5'-C5'	-7.35	109.88	120.90
1	y	120	THR	N-CA-C	-7.34	101.47	112.04
11	5	2099	U	C4'-C3'-C2'	-7.34	95.26	102.60
10	4	1870	C	O4'-C4'-C3'	-7.33	98.77	106.10
1	y	205	HIS	ND1-CE1-NE2	7.33	115.73	108.40
10	4	1870	C	C5'-C4'-O4'	7.33	120.09	109.10
11	5	2171	A	C3'-C2'-C1'	-7.32	94.18	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	y	275	ILE	CA-C-O	-7.31	113.15	118.71
7	1	57	C	O4'-C1'-N1	7.31	119.47	108.50
6	Y	10	SER	CA-C-N	7.30	130.02	120.60
6	Y	10	SER	C-N-CA	7.30	130.02	120.60
1	y	270	ASN	N-CA-CB	7.30	122.83	110.49
2	E	80	ARG	NE-CZ-NH1	7.30	128.80	121.50
2	E	118	LEU	N-CA-CB	7.29	121.06	110.20
1	y	206	THR	N-CA-C	7.24	119.17	111.28
10	4	1874	C	O4'-C1'-N1	7.22	119.34	108.50
1	y	150	ILE	N-CA-C	-7.22	97.50	107.75
8	2	1325	U	O3'-P-O5'	-7.18	93.23	104.00
11	5	2110	G	P-O3'-C3'	7.17	130.96	120.20
1	y	372	ARG	NE-CZ-NH1	-7.16	114.34	121.50
11	5	2095	A	P-O5'-C5'	-7.13	110.20	120.90
6	Y	51	ALA	CA-C-N	7.13	131.51	120.82
6	Y	51	ALA	C-N-CA	7.13	131.51	120.82
11	5	2166	U	C4'-C3'-C2'	-7.10	95.50	102.60
1	y	198	GLY	CA-C-N	7.09	129.77	120.26
1	y	198	GLY	C-N-CA	7.09	129.77	120.26
1	y	330	PHE	CA-C-N	7.09	130.09	120.44
1	y	330	PHE	C-N-CA	7.09	130.09	120.44
1	y	377	GLY	CA-C-N	7.08	129.78	120.28
1	y	377	GLY	C-N-CA	7.08	129.78	120.28
1	y	422	THR	N-CA-C	7.08	119.07	111.36
11	5	2132	U	O4'-C1'-N1	7.07	118.81	108.20
5	U	98	ASN	N-CA-C	-7.06	105.59	114.56
8	2	1335	C	P-O3'-C3'	7.06	130.78	120.20
1	y	180	GLU	O-C-N	7.05	129.71	122.09
9	3	1527	G	P-O3'-C3'	7.04	130.76	120.20
1	y	220	LEU	CA-C-N	7.02	129.69	120.28
1	y	220	LEU	C-N-CA	7.02	129.69	120.28
1	y	173	TRP	N-CA-C	-7.02	103.71	112.90
4	T	66	LYS	N-CA-C	-7.02	95.57	107.99
1	y	166	THR	CA-CB-CG2	7.00	122.40	110.50
3	G	52	MET	N-CA-C	-7.00	95.89	110.80
1	y	216	HIS	CA-CB-CG	-6.99	106.81	113.80
11	5	2176	A	C5'-C4'-C3'	-6.97	105.54	116.00
5	U	14	THR	CA-C-N	6.96	127.41	120.31
5	U	14	THR	C-N-CA	6.96	127.41	120.31
1	y	390	PHE	N-CA-C	6.95	118.93	111.36
1	y	30	LEU	CA-C-N	6.91	129.40	120.56
1	y	30	LEU	C-N-CA	6.91	129.40	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	5	2111	U	P-O5'-C5'	6.91	131.26	120.90
7	1	63	A	C5'-C4'-C3'	-6.88	105.68	116.00
6	Y	25	GLN	N-CA-C	-6.86	104.06	113.18
1	y	325	ILE	N-CA-C	6.85	117.00	110.42
2	E	81	LYS	N-CA-CB	6.85	121.21	110.46
1	y	307	SER	CA-C-N	6.83	129.43	120.28
1	y	307	SER	C-N-CA	6.83	129.43	120.28
2	E	105	SER	CA-C-O	6.82	127.81	119.97
1	y	226	LEU	CA-C-N	6.79	129.12	120.56
1	y	226	LEU	C-N-CA	6.79	129.12	120.56
1	y	417	MET	N-CA-C	-6.79	104.20	113.30
11	5	2115	G	P-O5'-C5'	-6.78	110.73	120.90
1	y	369	VAL	CA-C-N	6.78	129.36	120.28
1	y	369	VAL	C-N-CA	6.78	129.36	120.28
1	y	177	GLN	N-CA-C	6.78	118.67	111.28
6	Y	32	ALA	N-CA-C	6.75	118.64	111.28
6	Y	30	MET	CA-C-N	6.75	129.21	120.44
6	Y	30	MET	C-N-CA	6.75	129.21	120.44
1	y	162	VAL	CA-C-N	6.74	129.21	120.44
1	y	162	VAL	C-N-CA	6.74	129.21	120.44
10	4	1870	C	C1'-O4'-C4'	6.72	116.42	109.70
1	y	130	PHE	CA-C-O	-6.72	113.42	120.55
5	U	36	GLU	N-CA-CB	6.71	119.85	109.85
4	T	5	GLU	CB-CG-CD	-6.70	101.22	112.60
8	2	1324	G	P-O5'-C5'	-6.68	110.87	120.90
1	y	320	LEU	N-CA-C	-6.68	105.28	113.50
11	5	2111	U	P-O3'-C3'	6.66	130.19	120.20
1	y	93	GLN	N-CA-C	6.65	119.36	111.71
7	1	79	C	O4'-C1'-N1	6.64	118.46	108.50
11	5	2097	A	C4'-C3'-C2'	-6.64	95.96	102.60
1	y	41	ILE	CA-C-N	6.63	128.01	120.85
1	y	41	ILE	C-N-CA	6.63	128.01	120.85
1	y	288	ALA	CB-CA-C	-6.63	100.47	110.88
11	5	2174	C	O4'-C1'-N1	6.63	118.44	108.50
9	3	1531	C	P-O3'-C3'	6.61	130.12	120.20
11	5	2175	C	P-O3'-C3'	6.61	130.12	120.20
10	4	1898	U	P-O5'-C5'	6.61	130.81	120.90
7	1	83	A	P-O5'-C5'	6.60	130.81	120.90
1	y	79	ALA	CA-C-N	6.58	129.00	120.44
1	y	79	ALA	C-N-CA	6.58	129.00	120.44
2	E	112	ASP	CA-CB-CG	-6.58	106.02	112.60
10	4	1852	U	O4'-C1'-N1	6.57	118.35	108.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Y	11	VAL	CA-C-O	-6.57	114.44	121.27
5	U	44	HIS	CE1-NE2-CD2	-6.55	102.45	109.00
1	y	317	TYR	N-CA-CB	6.55	120.18	110.49
9	3	1533	C	O4'-C1'-N1	6.53	118.30	108.50
8	2	1333	G	C3'-C2'-C1'	6.51	107.81	101.30
5	U	9	GLU	O-C-N	-6.49	115.60	123.19
6	Y	11	VAL	N-CA-C	6.49	117.17	110.36
11	5	2177	C	O4'-C1'-N1	6.49	118.23	108.50
11	5	2116	G	C1'-O4'-C4'	-6.48	103.22	109.70
7	1	111	A	O4'-C1'-N9	6.48	118.22	108.50
1	y	60	ILE	CA-C-N	6.47	129.66	120.53
1	y	60	ILE	C-N-CA	6.47	129.66	120.53
1	y	417	MET	O-C-N	-6.47	114.41	122.24
1	y	74	ARG	NE-CZ-NH2	-6.44	113.40	119.20
7	1	76	C	O5'-C5'-C4'	-6.44	101.84	111.50
11	5	2118	U	P-O3'-C3'	-6.44	110.54	120.20
1	y	215	LEU	N-CA-C	-6.44	97.09	110.80
1	y	71	ALA	N-CA-C	-6.44	105.46	113.38
1	y	176	GLU	N-CA-C	6.44	119.29	111.82
1	y	62	GLU	CA-C-N	6.43	129.22	120.54
1	y	62	GLU	C-N-CA	6.43	129.22	120.54
1	y	414	MET	CA-C-N	6.42	128.79	120.44
1	y	414	MET	C-N-CA	6.42	128.79	120.44
11	5	2102	G	O4'-C1'-N9	6.40	118.11	108.50
8	2	1327	A	P-O5'-C5'	-6.40	111.30	120.90
8	2	1342	A	O4'-C4'-C3'	-6.38	99.72	106.10
5	U	36	GLU	CB-CA-C	-6.38	99.68	109.89
6	Y	31	GLN	CA-C-N	6.38	128.82	120.28
6	Y	31	GLN	C-N-CA	6.38	128.82	120.28
11	5	2183	A	C4'-C3'-C2'	-6.35	96.25	102.60
10	4	1863	G	P-O5'-C5'	-6.34	111.39	120.90
11	5	2106	U	C4'-C3'-O3'	-6.34	103.49	113.00
1	y	340	ARG	NE-CZ-NH1	-6.34	115.16	121.50
11	5	2146	C	O4'-C1'-N1	6.33	117.99	108.50
3	G	45	SER	N-CA-CB	-6.33	99.80	110.49
2	E	94	THR	N-CA-C	-6.33	105.60	113.38
1	y	140	PRO	N-CA-C	-6.32	106.59	114.68
5	U	96	LYS	CA-C-O	6.32	126.63	119.18
5	U	13	LEU	N-CA-C	-6.32	104.84	113.30
1	y	256	ARG	CA-C-N	6.31	129.28	121.71
1	y	256	ARG	C-N-CA	6.31	129.28	121.71
6	Y	24	GLU	O-C-N	-6.31	114.20	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	80	ARG	N-CA-C	6.29	119.11	111.82
1	y	287	PRO	N-CA-CB	6.28	110.48	103.44
1	y	39	ILE	N-CA-C	-6.28	100.88	107.60
6	Y	35	GLY	CA-C-N	6.28	129.20	120.29
6	Y	35	GLY	C-N-CA	6.28	129.20	120.29
10	4	1861	G	O4'-C1'-N9	6.27	117.91	108.50
1	y	338	ASN	O-C-N	-6.27	114.11	121.32
4	T	18	GLU	CA-C-N	6.27	129.74	120.90
4	T	18	GLU	C-N-CA	6.27	129.74	120.90
1	y	150	ILE	O-C-N	-6.26	116.16	122.67
1	y	286	PHE	CA-C-N	6.25	125.67	118.85
1	y	286	PHE	C-N-CA	6.25	125.67	118.85
7	1	71	A	O4'-C1'-C2'	6.25	112.05	105.80
1	y	104	GLU	CA-C-N	6.24	128.42	120.56
1	y	104	GLU	C-N-CA	6.24	128.42	120.56
2	E	84	TRP	CA-CB-CG	6.24	125.45	113.60
11	5	2127	G	P-O3'-C3'	-6.23	110.86	120.20
1	y	291	ALA	N-CA-CB	6.22	119.26	110.12
1	y	386	LEU	N-CA-CB	6.21	120.51	110.40
2	E	123	THR	CA-C-N	6.18	126.81	119.94
2	E	123	THR	C-N-CA	6.18	126.81	119.94
11	5	2178	C	O4'-C1'-N1	6.18	117.77	108.50
3	G	55	MET	N-CA-C	-6.17	104.66	111.82
1	y	328	PHE	N-CA-C	6.16	117.99	111.28
11	5	2167	U	P-O5'-C5'	6.15	130.13	120.90
1	y	85	TYR	CB-CG-CD1	-6.15	111.57	120.80
1	y	64	PHE	CA-C-N	6.15	129.66	120.31
1	y	64	PHE	C-N-CA	6.15	129.66	120.31
4	T	1	MET	CA-C-N	6.15	129.60	122.35
4	T	1	MET	C-N-CA	6.15	129.60	122.35
1	y	261	GLN	N-CA-C	-6.14	99.85	109.25
10	4	1874	C	C4'-C3'-C2'	-6.14	96.46	102.60
3	G	45	SER	CB-CA-C	6.14	122.63	110.42
1	y	387	ILE	CA-C-N	6.13	126.31	119.32
1	y	387	ILE	C-N-CA	6.13	126.31	119.32
10	4	1848	A	C4'-C3'-C2'	-6.13	96.47	102.60
7	1	87	U	O5'-C5'-C4'	-6.12	102.31	111.50
1	y	308	LEU	CA-C-O	-6.11	114.07	120.55
7	1	57	C	O4'-C1'-C2'	-6.11	101.49	107.60
1	y	81	GLY	CA-C-N	6.11	130.32	120.30
1	y	81	GLY	C-N-CA	6.11	130.32	120.30
1	y	400	TYR	O-C-N	-6.09	116.61	123.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	43	ILE	CB-CA-C	-6.09	103.06	111.65
7	1	56	A	O4'-C1'-N9	6.09	117.63	108.50
6	Y	9	LYS	CA-C-N	6.07	133.13	121.54
6	Y	9	LYS	C-N-CA	6.07	133.13	121.54
4	T	77	ARG	CA-C-N	6.07	133.12	121.54
4	T	77	ARG	C-N-CA	6.07	133.12	121.54
11	5	2167	U	O4'-C1'-N1	6.07	117.60	108.50
6	Y	17	GLU	CA-C-N	6.06	128.69	120.38
6	Y	17	GLU	C-N-CA	6.06	128.69	120.38
4	T	72	GLN	CA-C-O	6.06	126.94	120.10
8	2	1337	G	P-O5'-C5'	-6.04	111.83	120.90
1	y	11	SER	CA-C-N	6.03	128.36	120.28
1	y	11	SER	C-N-CA	6.03	128.36	120.28
7	1	62	U	P-O3'-C3'	6.03	129.24	120.20
1	y	182	GLY	CA-C-N	6.03	132.82	121.97
1	y	182	GLY	C-N-CA	6.03	132.82	121.97
11	5	2172	U	O4'-C4'-C3'	-6.01	100.09	106.10
1	y	261	GLN	OE1-CD-NE2	6.01	128.61	122.60
5	U	4	ILE	CA-CB-CG1	6.01	120.62	110.40
8	2	1333	G	P-O5'-C5'	6.01	129.91	120.90
5	U	90	LYS	N-CA-CB	6.00	120.69	111.56
3	G	50	ASN	N-CA-C	-6.00	97.33	108.02
1	y	287	PRO	O-C-N	6.00	129.73	122.23
1	y	410	VAL	CA-C-O	-6.00	114.50	120.85
11	5	2168	G	P-O5'-C5'	5.98	129.87	120.90
1	y	215	LEU	CA-C-N	5.97	130.84	120.68
1	y	215	LEU	C-N-CA	5.97	130.84	120.68
1	y	257	VAL	N-CA-C	-5.96	107.69	113.53
10	4	1845	G	O4'-C1'-N9	5.96	117.44	108.50
4	T	19	LYS	CG-CD-CE	5.95	124.99	111.30
4	T	79	ASP	N-CA-CB	5.95	118.76	110.26
1	y	56	GLN	OE1-CD-NE2	5.94	128.54	122.60
11	5	2158	A	C4'-C3'-C2'	-5.94	96.66	102.60
11	5	2126	A	P-O5'-C5'	-5.94	111.99	120.90
1	y	57	ARG	CA-C-O	5.93	125.73	119.03
11	5	2147	A	P-O5'-C5'	5.93	129.80	120.90
1	y	203	ILE	N-CA-C	5.92	117.37	110.62
6	Y	52	ARG	NE-CZ-NH2	5.92	124.53	119.20
8	2	1342	A	C5'-C4'-O4'	5.91	117.97	109.10
5	U	92	VAL	N-CA-CB	5.91	121.13	111.44
10	4	1896	G	C4'-C3'-O3'	-5.91	104.14	113.00
7	1	73	A	C4'-C3'-O3'	-5.90	104.14	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	y	39	ILE	CA-C-N	5.90	127.22	119.84
1	y	39	ILE	C-N-CA	5.90	127.22	119.84
3	G	56	THR	N-CA-C	-5.90	104.77	111.14
11	5	2119	A	C4'-C3'-O3'	5.90	118.25	109.40
1	y	35	ILE	CA-CB-CG1	-5.89	100.38	110.40
1	y	99	HIS	ND1-CG-CD2	5.89	112.00	106.10
1	y	433	LEU	CA-C-N	5.89	128.10	120.44
1	y	433	LEU	C-N-CA	5.89	128.10	120.44
1	y	192	PHE	CA-C-N	5.89	128.17	120.28
1	y	192	PHE	C-N-CA	5.89	128.17	120.28
4	T	89	GLU	CA-C-N	5.89	132.95	121.41
4	T	89	GLU	C-N-CA	5.89	132.95	121.41
7	1	97	C	O4'-C1'-N1	5.88	117.32	108.50
6	Y	46	VAL	CA-C-N	5.87	128.07	120.44
6	Y	46	VAL	C-N-CA	5.87	128.07	120.44
10	4	1871	A	P-O3'-C3'	5.87	129.01	120.20
8	2	1314	C	O4'-C1'-C2'	-5.87	101.73	107.60
6	Y	53	VAL	CA-C-O	-5.86	114.86	120.95
8	2	1342	A	C3'-C2'-C1'	-5.86	95.64	101.50
1	y	151	ASN	CA-C-N	5.85	125.86	119.89
1	y	151	ASN	C-N-CA	5.85	125.86	119.89
1	y	316	LEU	N-CA-C	-5.85	105.64	112.89
1	y	430	GLU	N-CA-CB	5.85	118.49	110.01
1	y	102	LEU	CA-C-N	5.84	128.03	120.44
1	y	102	LEU	C-N-CA	5.84	128.03	120.44
1	y	216	HIS	ND1-CE1-NE2	5.84	114.24	108.40
1	y	433	LEU	N-CA-CB	5.83	119.28	110.30
2	E	86	THR	N-CA-CB	5.82	119.35	110.44
6	Y	46	VAL	N-CA-CB	5.82	120.83	111.23
7	1	84	A	C5'-C4'-O4'	5.82	117.83	109.10
5	U	60	LYS	CA-C-N	5.82	129.63	121.02
5	U	60	LYS	C-N-CA	5.82	129.63	121.02
1	y	87	SER	CA-C-O	-5.81	114.26	120.42
1	y	137	THR	CA-C-N	5.81	126.39	119.94
1	y	137	THR	C-N-CA	5.81	126.39	119.94
1	y	423	LEU	CA-C-N	5.81	128.07	120.28
1	y	423	LEU	C-N-CA	5.81	128.07	120.28
1	y	163	SER	N-CA-CB	5.81	118.44	110.01
1	y	194	GLY	CA-C-O	-5.81	114.39	120.90
6	Y	18	LEU	CA-C-O	5.81	126.90	120.63
1	y	45	ASP	N-CA-CB	5.81	120.93	110.83
6	Y	7	ARG	CA-C-O	-5.79	112.27	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	5	2104	C	C3'-C2'-O2'	5.79	119.39	110.70
10	4	1893	C	O4'-C1'-N1	5.79	117.18	108.50
1	y	258	TYR	N-CA-CB	5.78	120.26	110.49
10	4	1843	C	O4'-C1'-N1	5.78	117.17	108.50
7	1	112	U	O4'-C1'-N1	5.78	117.17	108.50
10	4	1881	C	C3'-C2'-O2'	5.77	119.36	110.70
1	y	60	ILE	N-CA-C	5.77	116.42	110.36
10	4	1870	C	O4'-C1'-N1	5.77	116.85	108.20
8	2	1323	C	O4'-C1'-N1	5.76	117.14	108.50
9	3	1532	A	C4'-C3'-O3'	-5.76	104.36	113.00
1	y	97	VAL	O-C-N	5.75	127.45	121.87
1	y	99	HIS	CB-CG-CD2	-5.75	123.72	131.20
1	y	170	PHE	CA-C-N	5.75	127.98	120.28
1	y	170	PHE	C-N-CA	5.75	127.98	120.28
7	1	60	G	C2'-C3'-O3'	5.75	118.12	109.50
7	1	102	U	P-O3'-C3'	5.74	128.80	120.20
6	Y	36	GLN	OE1-CD-NE2	-5.73	116.87	122.60
4	T	82	LYS	N-CA-C	-5.73	100.37	109.59
1	y	395	MET	O-C-N	-5.72	115.41	122.68
7	1	88	G	C4'-C3'-O3'	-5.72	104.42	113.00
11	5	2159	G	O4'-C1'-C2'	-5.71	101.89	107.60
10	4	1876	A	C4'-C3'-C2'	5.71	108.31	102.60
11	5	2106	U	C4'-C3'-C2'	-5.71	96.89	102.60
1	y	21	ARG	NE-CZ-NH1	5.71	127.21	121.50
1	y	119	TYR	CA-CB-CG	5.70	124.16	113.90
7	1	63	A	O4'-C1'-N9	5.70	117.04	108.50
1	y	117	SER	CA-C-N	5.69	127.90	120.28
1	y	117	SER	C-N-CA	5.69	127.90	120.28
4	T	77	ARG	NE-CZ-NH2	-5.69	114.08	119.20
6	Y	27	ASN	CA-C-N	5.69	127.83	120.44
6	Y	27	ASN	C-N-CA	5.69	127.83	120.44
2	E	117	ARG	NE-CZ-NH2	-5.69	114.08	119.20
5	U	20	LYS	CA-C-O	-5.68	114.02	120.32
4	T	28	ASN	CA-C-N	5.67	132.37	121.54
4	T	28	ASN	C-N-CA	5.67	132.37	121.54
1	y	72	LEU	N-CA-C	-5.66	106.73	113.97
11	5	2188	U	C4'-C3'-O3'	-5.66	104.51	113.00
11	5	2126	A	C2'-C3'-O3'	5.65	117.97	109.50
7	1	90	U	O4'-C1'-N1	5.64	116.97	108.50
1	y	243	ARG	NE-CZ-NH1	5.64	127.14	121.50
1	y	227	VAL	N-CA-CB	5.64	117.15	110.55
1	y	144	GLY	N-CA-C	-5.63	102.41	111.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	15	HIS	CE1-NE2-CD2	-5.63	103.37	109.00
5	U	86	PHE	CB-CG-CD1	5.63	130.27	120.70
11	5	2173	A	O4'-C4'-C3'	5.62	109.62	104.00
11	5	2193	G	O4'-C1'-N9	5.62	116.94	108.50
10	4	1842	G	P-O5'-C5'	-5.62	112.47	120.90
10	4	1860	G	C1'-C2'-O2'	5.62	116.83	108.40
1	y	427	SER	CA-C-N	5.61	127.74	120.44
1	y	427	SER	C-N-CA	5.61	127.74	120.44
5	U	24	VAL	N-CA-CB	5.61	117.73	111.89
1	y	304	THR	CA-C-N	5.61	127.80	120.28
1	y	304	THR	C-N-CA	5.61	127.80	120.28
11	5	2182	U	C5'-C4'-C3'	-5.61	107.59	116.00
8	2	1312	U	C1'-O4'-C4'	-5.60	104.10	109.70
1	y	200	PRO	CA-C-O	-5.60	112.44	120.56
1	y	231	THR	N-CA-C	5.60	118.15	111.71
5	U	35	VAL	CA-C-N	5.60	128.79	120.95
5	U	35	VAL	C-N-CA	5.60	128.79	120.95
6	Y	29	ARG	CG-CD-NE	-5.60	99.69	112.00
11	5	2177	C	C5'-C4'-O4'	5.60	118.20	109.80
7	1	56	A	O4'-C1'-C2'	-5.59	102.01	107.60
2	E	96	ILE	CA-C-O	-5.59	115.25	121.17
1	y	345	ASN	CB-CA-C	-5.58	102.08	110.90
2	E	124	GLY	O-C-N	5.58	127.53	122.18
6	Y	32	ALA	CB-CA-C	-5.58	101.53	110.79
1	y	123	GLY	CA-C-N	5.56	128.19	120.29
1	y	123	GLY	C-N-CA	5.56	128.19	120.29
1	y	181	ARG	NE-CZ-NH1	-5.56	115.94	121.50
1	y	396	LYS	O-C-N	-5.56	115.20	122.59
1	y	379	LEU	CA-C-N	5.55	128.18	120.29
1	y	379	LEU	C-N-CA	5.55	128.18	120.29
1	y	181	ARG	CB-CA-C	-5.55	101.58	110.79
11	5	2181	U	O4'-C1'-N1	5.54	116.81	108.50
1	y	346	LEU	CA-C-N	5.54	127.64	120.44
1	y	346	LEU	C-N-CA	5.54	127.64	120.44
1	y	381	ILE	N-CA-CB	5.53	116.65	110.51
6	Y	11	VAL	CA-C-N	5.53	127.95	120.65
6	Y	11	VAL	C-N-CA	5.53	127.95	120.65
1	y	47	ALA	CA-C-O	-5.51	114.71	120.55
1	y	434	LYS	N-CA-CB	5.51	118.00	110.01
11	5	2123	G	O4'-C1'-N9	5.51	116.77	108.50
11	5	2147	A	C3'-C2'-C1'	-5.50	95.80	101.30
1	y	135	ILE	N-CA-C	-5.50	105.36	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	y	162	VAL	N-CA-C	-5.49	105.15	110.42
7	1	57	C	O4'-C4'-C3'	-5.49	98.51	104.00
3	G	65	ILE	N-CA-C	-5.49	104.36	112.04
1	y	122	TYR	O-C-N	5.48	128.40	122.15
11	5	2139	U	O4'-C1'-N1	5.48	116.72	108.50
5	U	77	GLY	CA-C-N	5.48	128.49	120.71
5	U	77	GLY	C-N-CA	5.48	128.49	120.71
7	1	73	A	P-O3'-C3'	-5.47	111.99	120.20
8	2	1328	A	P-O5'-C5'	5.47	129.11	120.90
11	5	2125	G	C1'-O4'-C4'	-5.47	104.43	109.90
1	y	375	LEU	N-CA-C	-5.47	105.24	111.14
1	y	46	ALA	N-CA-C	5.46	117.23	111.28
6	Y	48	ARG	NH1-CZ-NH2	-5.46	112.20	119.30
7	1	60	G	O4'-C1'-C2'	5.46	111.26	105.80
1	y	360	GLU	CA-C-N	5.45	128.59	120.31
1	y	360	GLU	C-N-CA	5.45	128.59	120.31
2	E	85	PRO	O-C-N	-5.45	114.91	122.37
7	1	53	A	O4'-C1'-N9	5.45	116.67	108.50
1	y	228	PHE	N-CA-CB	5.44	118.12	110.12
9	3	1537	G	P-O3'-C3'	5.44	128.36	120.20
1	y	101	THR	N-CA-C	5.43	116.88	111.07
1	y	312	PRO	N-CA-C	5.43	119.72	111.15
5	U	80	ASP	N-CA-CB	5.42	119.66	110.49
7	1	84	A	C5'-C4'-C3'	-5.42	107.07	115.20
5	U	82	VAL	O-C-N	-5.42	117.61	123.14
1	y	10	GLN	N-CA-CB	5.42	118.08	110.12
5	U	102	ILE	N-CA-CB	5.42	118.89	111.41
11	5	2173	A	C3'-C2'-O2'	5.42	118.83	110.70
8	2	1327	A	C3'-C2'-O2'	5.41	118.82	110.70
1	y	188	SER	CA-C-O	-5.41	113.41	119.79
11	5	2140	G	O3'-P-O5'	-5.41	95.89	104.00
1	y	329	CYS	N-CA-C	5.41	117.17	111.28
10	4	1844	C	P-O5'-C5'	5.40	129.00	120.90
8	2	1325	U	O4'-C1'-N1	5.40	116.30	108.20
5	U	10	VAL	CA-C-O	5.39	127.52	120.78
1	y	232	PHE	O-C-N	5.39	127.62	122.07
1	y	423	LEU	N-CA-C	5.39	116.96	111.14
1	y	46	ALA	CB-CA-C	-5.39	101.85	110.79
1	y	98	VAL	CB-CA-C	-5.39	104.87	112.14
1	y	61	ILE	CA-C-O	-5.38	115.45	121.05
10	4	1891	G	P-O5'-C5'	5.38	128.98	120.90
4	T	34	VAL	CA-C-N	5.38	127.44	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	34	VAL	C-N-CA	5.38	127.44	120.44
5	U	30	SER	N-CA-C	-5.38	106.30	112.92
11	5	2140	G	O4'-C1'-C2'	-5.38	102.22	107.60
5	U	16	LYS	N-CA-C	-5.38	102.34	113.31
7	1	101	A	O4'-C1'-N9	5.37	116.56	108.50
1	y	131	GLN	CB-CA-C	-5.37	101.72	110.85
11	5	2177	C	C5'-C4'-C3'	-5.36	107.96	116.00
1	y	233	PHE	N-CA-CB	5.36	118.00	110.12
11	5	2171	A	O4'-C1'-N9	5.35	116.23	108.20
2	E	106	LEU	CB-CA-C	5.35	119.95	110.85
7	1	57	C	C1'-O4'-C4'	5.35	115.25	109.90
10	4	1872	A	O4'-C1'-N9	5.35	116.53	108.50
2	E	92	HIS	N-CA-C	-5.34	101.67	109.63
11	5	2184	A	O4'-C1'-N9	5.34	116.52	108.50
1	y	187	ILE	O-C-N	-5.34	116.68	121.91
8	2	1326	U	C5'-C4'-C3'	-5.34	108.00	116.00
1	y	35	ILE	N-CA-CB	5.33	117.40	110.57
6	Y	47	ARG	NE-CZ-NH1	-5.33	116.17	121.50
11	5	2108	A	O4'-C1'-N9	5.33	116.50	108.50
4	T	1	MET	CG-SD-CE	-5.33	89.18	100.90
6	Y	13	GLU	CA-C-N	5.33	127.73	120.54
6	Y	13	GLU	C-N-CA	5.33	127.73	120.54
11	5	2150	C	P-O3'-C3'	5.33	128.19	120.20
1	y	360	GLU	N-CA-C	5.32	117.98	111.82
9	3	1534	U	O4'-C1'-N1	5.31	116.47	108.50
4	T	84	TYR	N-CA-CB	5.31	118.65	110.21
11	5	2172	U	P-O5'-C5'	-5.31	112.93	120.90
11	5	2140	G	C3'-C2'-C1'	5.31	106.61	101.30
4	T	70	HIS	ND1-CE1-NE2	5.30	113.70	108.40
7	1	100	U	C5'-C4'-C3'	-5.30	107.24	115.20
11	5	2188	U	O4'-C1'-N1	5.30	116.46	108.50
5	U	80	ASP	CA-C-N	5.30	131.66	121.54
5	U	80	ASP	C-N-CA	5.30	131.66	121.54
8	2	1324	G	C5'-C4'-C3'	-5.30	107.25	115.20
6	Y	7	ARG	N-CA-C	-5.30	106.59	113.16
1	y	159	THR	CA-C-N	5.29	127.32	120.44
1	y	159	THR	C-N-CA	5.29	127.32	120.44
4	T	12	ARG	N-CA-C	-5.29	105.89	114.09
5	U	49	PRO	N-CA-CB	5.29	108.80	103.25
6	Y	53	VAL	N-CA-C	5.29	116.02	110.62
2	E	111	LEU	CB-CA-C	-5.29	101.03	110.70
5	U	19	GLY	CA-C-O	5.29	125.70	119.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	U	49	PRO	CA-N-CD	-5.29	104.60	112.00
9	3	1540	G	N1-C6-O6	5.28	135.75	119.90
1	y	32	VAL	CA-C-O	5.28	126.17	120.47
7	1	99	U	O4'-C4'-C3'	-5.28	98.72	104.00
11	5	2172	U	C5'-C4'-C3'	5.28	123.12	115.20
9	3	1528	A	C4'-C3'-C2'	-5.28	97.32	102.60
11	5	2160	C	O5'-C5'-C4'	-5.28	103.59	111.50
11	5	2176	A	O4'-C1'-C2'	-5.27	102.33	107.60
11	5	2188	U	P-O3'-C3'	-5.27	112.29	120.20
1	y	142	MET	CA-C-O	-5.26	112.95	120.16
4	T	32	LEU	CD1-CG-CD2	-5.26	99.23	110.80
1	y	236	PHE	CB-CG-CD2	-5.25	111.77	120.70
1	y	288	ALA	CA-C-N	5.24	127.73	120.29
1	y	288	ALA	C-N-CA	5.24	127.73	120.29
1	y	74	ARG	N-CA-C	-5.24	101.16	109.59
8	2	1318	U	O4'-C1'-N1	5.24	116.36	108.50
7	1	57	C	C4'-C3'-C2'	-5.24	97.36	102.60
8	2	1310	G	C5'-C4'-C3'	-5.23	108.16	116.00
1	y	14	GLY	CA-C-N	5.23	125.78	119.98
1	y	14	GLY	C-N-CA	5.23	125.78	119.98
6	Y	2	LYS	CA-C-N	5.23	127.81	120.28
6	Y	2	LYS	C-N-CA	5.23	127.81	120.28
7	1	72	U	C1'-O4'-C4'	-5.23	104.47	109.70
1	y	185	ASN	CA-CB-CG	-5.22	107.38	112.60
6	Y	24	GLU	CA-C-O	5.22	127.98	120.51
5	U	14	THR	CA-C-O	5.22	126.44	120.54
11	5	2198	A	N1-C6-N6	5.22	134.26	118.60
1	y	228	PHE	CA-C-O	-5.21	115.02	120.55
2	E	91	LEU	N-CA-C	-5.21	100.23	108.14
7	1	78	U	P-O5'-C5'	5.21	128.71	120.90
1	y	162	VAL	CB-CA-C	-5.21	105.31	111.97
4	T	25	GLU	CG-CD-OE2	-5.20	106.44	118.40
7	1	112	U	C1'-O4'-C4'	-5.20	104.70	109.90
4	T	34	VAL	N-CA-C	-5.20	99.02	107.28
5	U	65	GLN	O-C-N	-5.20	116.55	122.68
11	5	2168	G	P-O3'-C3'	-5.20	112.41	120.20
9	3	1531	C	C4'-C3'-O3'	-5.20	105.21	113.00
11	5	2101	A	C4'-C3'-C2'	-5.19	97.41	102.60
11	5	2153	C	O4'-C4'-C3'	-5.19	100.91	106.10
1	y	419	GLN	OE1-CD-NE2	5.19	127.79	122.60
1	y	410	VAL	N-CA-CB	5.19	118.36	110.58
9	3	1541	C	O4'-C1'-N1	5.18	116.28	108.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	4	1887	C	C4'-C3'-C2'	-5.18	97.42	102.60
8	2	1319	C	O4'-C1'-N1	5.18	116.27	108.50
11	5	2165	C	C4'-C3'-O3'	-5.18	105.23	113.00
1	y	407	LEU	O-C-N	5.18	127.61	122.12
1	y	139	LEU	CA-C-O	-5.17	113.66	118.73
1	y	418	ALA	CA-C-N	5.17	127.21	120.28
1	y	418	ALA	C-N-CA	5.17	127.21	120.28
7	1	52	A	P-O3'-C3'	-5.17	112.45	120.20
8	2	1308	A	P-O3'-C3'	5.17	127.95	120.20
9	3	1542	U	O4'-C1'-N1	5.17	116.25	108.50
11	5	2181	U	C1'-O4'-C4'	-5.16	104.74	109.90
11	5	2155	U	P-O5'-C5'	-5.16	113.16	120.90
5	U	64	ILE	CA-C-N	5.16	130.13	120.95
5	U	64	ILE	C-N-CA	5.16	130.13	120.95
5	U	48	VAL	CA-CB-CG2	-5.16	101.63	110.40
6	Y	3	ALA	N-CA-CB	5.16	118.16	110.22
1	y	373	LEU	N-CA-C	5.15	116.58	111.07
5	U	47	PRO	N-CD-CG	5.15	110.93	103.20
1	y	15	GLY	N-CA-C	5.15	118.91	112.73
1	y	428	GLN	CB-CA-C	-5.14	102.80	110.88
1	y	248	TYR	CA-C-N	5.14	131.36	121.54
1	y	248	TYR	C-N-CA	5.14	131.36	121.54
1	y	324	ALA	N-CA-C	5.14	116.88	111.28
1	y	179	THR	O-C-N	5.14	127.56	122.12
7	1	108	G	P-O5'-C5'	5.13	128.60	120.90
10	4	1847	A	O4'-C1'-N9	5.13	116.20	108.50
2	E	76	ARG	CA-CB-CG	5.13	124.36	114.10
11	5	2129	C	O4'-C1'-N1	5.13	115.89	108.20
10	4	1838	C	C4'-C3'-C2'	-5.13	97.47	102.60
11	5	2093	G	C3'-C2'-O2'	5.13	118.39	110.70
2	E	118	LEU	CB-CA-C	-5.13	101.32	110.70
11	5	2155	U	O4'-C1'-N1	5.13	116.19	108.50
11	5	2181	U	O5'-C5'-C4'	-5.13	103.81	111.50
1	y	8	ASP	CA-C-N	5.12	128.09	120.31
1	y	8	ASP	C-N-CA	5.12	128.09	120.31
1	y	161	VAL	CA-CB-CG2	-5.11	101.71	110.40
10	4	1883	U	O3'-P-O5'	-5.11	96.33	104.00
1	y	283	ILE	N-CA-C	5.11	115.83	110.62
1	y	131	GLN	CA-C-O	-5.11	115.01	120.42
4	T	76	ARG	CD-NE-CZ	-5.11	117.25	124.40
11	5	2132	U	N1-C1'-C2'	-5.10	106.35	114.00
5	U	66	VAL	CB-CA-C	-5.10	102.80	111.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	5	2164	C	C3'-C2'-C1'	-5.10	96.40	101.50
5	U	44	HIS	CG-CD2-NE2	5.09	112.29	107.20
7	1	96	C	C4'-C3'-O3'	-5.09	105.36	113.00
11	5	2150	C	N1-C1'-C2'	-5.09	104.36	112.00
1	y	25	PHE	CA-C-O	-5.09	113.79	119.79
1	y	291	ALA	CA-C-N	5.09	127.35	120.38
1	y	291	ALA	C-N-CA	5.09	127.35	120.38
11	5	2183	A	O3'-P-O5'	-5.08	96.38	104.00
1	y	10	GLN	N-CA-C	5.08	116.82	111.28
11	5	2157	G	O4'-C1'-C2'	-5.07	102.53	107.60
2	E	88	GLN	N-CA-CB	5.07	119.06	110.49
10	4	1879	C	O4'-C1'-N1	5.07	116.10	108.50
7	1	73	A	O4'-C1'-N9	5.06	116.09	108.50
11	5	2132	U	C3'-C2'-O2'	-5.06	107.00	114.60
11	5	2180	U	C4'-C3'-O3'	-5.06	105.41	113.00
1	y	191	ILE	CA-C-O	5.06	126.22	120.85
1	y	206	THR	CA-CB-OG1	5.06	117.19	109.60
11	5	2151	U	O4'-C1'-N1	5.05	116.08	108.50
2	E	116	VAL	CA-CB-CG2	-5.05	101.81	110.40
5	U	48	VAL	CB-CA-C	5.05	116.12	110.52
8	2	1333	G	O4'-C1'-C2'	-5.05	102.55	107.60
1	y	35	ILE	CA-CB-CG2	5.04	119.06	110.50
1	y	380	TYR	N-CA-C	-5.04	105.87	111.36
7	1	53	A	O3'-P-O5'	5.04	111.55	104.00
11	5	2131	U	O4'-C4'-C3'	-5.04	101.06	106.10
1	y	142	MET	O-C-N	-5.03	115.54	121.32
6	Y	47	ARG	CB-CA-C	-5.03	102.99	110.88
1	y	254	GLY	O-C-N	5.02	129.23	122.70
6	Y	49	ASP	N-CA-C	-5.02	100.10	110.80
11	5	2124	G	C4'-C3'-C2'	-5.02	97.58	102.60
8	2	1310	G	C1'-C2'-O2'	5.00	115.91	108.40
5	U	70	ALA	CA-C-N	5.00	127.30	120.35
5	U	70	ALA	C-N-CA	5.00	127.30	120.35
7	1	86	G	P-O3'-C3'	5.00	127.70	120.20

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	G	45	SER	CA
3	G	48	SER	CA
3	G	51	PHE	CA

All (141) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	1	100	U	Sidechain
7	1	103	A	Sidechain
7	1	106	C	Sidechain
7	1	107	G	Sidechain
7	1	108	G	Sidechain
7	1	109	C	Sidechain
7	1	113	U	Sidechain
7	1	52	A	Sidechain
7	1	55	G	Sidechain
7	1	58	G	Sidechain
7	1	59	U	Sidechain
7	1	60	G	Sidechain
7	1	63	A	Sidechain
7	1	64	A	Sidechain
7	1	68	G	Sidechain
7	1	72	U	Sidechain
7	1	73	A	Sidechain
7	1	74	A	Sidechain
7	1	75	G	Sidechain
7	1	77	G	Sidechain
7	1	79	C	Sidechain
7	1	84	A	Sidechain
7	1	87	U	Sidechain
7	1	88	G	Sidechain
7	1	91	A	Sidechain
7	1	92	U	Sidechain
7	1	94	A	Sidechain
7	1	95	A	Sidechain
7	1	97	C	Sidechain
7	1	99	U	Sidechain
8	2	1310	G	Sidechain
8	2	1311	G	Sidechain
8	2	1312	U	Sidechain
8	2	1314	C	Sidechain
8	2	1324	G	Sidechain
8	2	1325	U	Sidechain
8	2	1326	U	Sidechain
8	2	1327	A	Sidechain
8	2	1328	A	Sidechain
8	2	1333	G	Sidechain
8	2	1334	G	Sidechain
8	2	1336	A	Sidechain

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Mol	Chain	Res	Type	Group
8	2	1337	G	Sidechain
8	2	1338	G	Sidechain
8	2	1341	G	Sidechain
9	3	1527	G	Sidechain
9	3	1529	G	Sidechain
9	3	1530	G	Sidechain
9	3	1534	U	Sidechain
9	3	1535	A	Sidechain
9	3	1537	G	Sidechain
9	3	1538	G	Sidechain
9	3	1539	U	Sidechain
9	3	1540	G	Sidechain
9	3	1542	U	Sidechain
10	4	1838	C	Sidechain
10	4	1840	G	Sidechain
10	4	1841	U	Sidechain
10	4	1846	G	Sidechain
10	4	1857	G	Sidechain
10	4	1858	A	Sidechain
10	4	1859	U	Sidechain
10	4	1860	G	Sidechain
10	4	1862	G	Sidechain
10	4	1864	U	Sidechain
10	4	1877	A	Sidechain
10	4	1878	G	Sidechain
10	4	1880	U	Sidechain
10	4	1881	C	Sidechain
10	4	1886	U	Sidechain
10	4	1887	C	Sidechain
10	4	1890	A	Sidechain
10	4	1891	G	Sidechain
10	4	1895	C	Sidechain
10	4	1898	U	Sidechain
11	5	2094	A	Sidechain
11	5	2099	U	Sidechain
11	5	2100	G	Sidechain
11	5	2101	A	Sidechain
11	5	2104	C	Sidechain
11	5	2105	U	Sidechain
11	5	2107	G	Sidechain
11	5	2110	G	Sidechain
11	5	2111	U	Sidechain

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Mol	Chain	Res	Type	Group
11	5	2113	U	Sidechain
11	5	2117	A	Sidechain
11	5	2119	A	Sidechain
11	5	2121	G	Sidechain
11	5	2123	G	Sidechain
11	5	2124	G	Sidechain
11	5	2125	G	Sidechain
11	5	2126	A	Sidechain
11	5	2127	G	Sidechain
11	5	2129	C	Sidechain
11	5	2130	U	Sidechain
11	5	2133	G	Sidechain
11	5	2139	U	Sidechain
11	5	2140	G	Sidechain
11	5	2142	A	Sidechain
11	5	2143	C	Sidechain
11	5	2146	C	Sidechain
11	5	2147	A	Sidechain
11	5	2148	G	Sidechain
11	5	2150	C	Sidechain
11	5	2151	U	Sidechain
11	5	2153	C	Sidechain
11	5	2157	G	Sidechain
11	5	2159	G	Sidechain
11	5	2160	C	Sidechain
11	5	2161	C	Sidechain
11	5	2162	G	Sidechain
11	5	2165	C	Sidechain
11	5	2169	A	Sidechain
11	5	2170	A	Sidechain
11	5	2171	A	Sidechain
11	5	2172	U	Sidechain
11	5	2174	C	Sidechain
11	5	2175	C	Sidechain
11	5	2179	C	Sidechain
11	5	2180	U	Sidechain
11	5	2182	U	Sidechain
11	5	2184	A	Sidechain
11	5	2187	U	Sidechain
11	5	2188	U	Sidechain
11	5	2189	U	Sidechain
11	5	2190	G	Sidechain

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Mol	Chain	Res	Type	Group
11	5	2192	U	Sidechain
11	5	2193	G	Sidechain
11	5	2194	U	Sidechain
2	E	92	HIS	Sidechain
4	T	77	ARG	Sidechain
5	U	48	VAL	Peptide
5	U	5	ARG	Sidechain
5	U	94	PHE	Sidechain
6	Y	26	PHE	Sidechain
1	y	216	HIS	Sidechain
1	y	248	TYR	Sidechain
1	y	25	PHE	Sidechain
1	y	309	TYR	Sidechain
1	y	390	PHE	Sidechain
1	y	400	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	y	3361	0	3514	157	0
2	E	433	0	466	30	0
3	G	457	0	481	109	0
4	T	787	0	846	17	0
5	U	789	0	847	4	0
6	Y	509	0	543	3	0
7	1	1350	0	676	8	0
8	2	775	0	385	19	0
9	3	387	0	196	0	0
10	4	1312	0	659	3	0
11	5	2305	0	1156	4	0
All	All	12465	0	9769	243	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 11.

All (243) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:355:GLY:O	1:y:356:ILE:CG1	1.82	1.28
1:y:354:PRO:O	1:y:356:ILE:N	1.68	1.24
2:E:126:ARG:HE	3:G:68:LEU:CD2	1.54	1.20
2:E:126:ARG:CB	3:G:68:LEU:HD21	1.73	1.18
1:y:352:PHE:CE1	8:2:1318:U:H4'	1.80	1.16
2:E:126:ARG:HE	3:G:68:LEU:HD22	1.02	1.08
2:E:126:ARG:NH2	3:G:65:ILE:HG12	1.68	1.08
1:y:39:ILE:CG2	3:G:68:LEU:HD13	1.82	1.08
1:y:355:GLY:O	1:y:356:ILE:HG13	0.90	1.07
1:y:353:VAL:HG22	1:y:354:PRO:HD2	1.36	1.07
1:y:162:VAL:HG22	3:G:19:LEU:HD21	1.36	1.06
1:y:352:PHE:CD1	8:2:1318:U:H4'	1.90	1.06
1:y:169:MET:SD	3:G:22:LEU:HD12	1.95	1.05
1:y:354:PRO:HA	1:y:357:ARG:CG	1.86	1.05
2:E:126:ARG:HB3	3:G:68:LEU:CD2	1.87	1.04
1:y:39:ILE:HG21	3:G:68:LEU:HD13	1.37	1.02
3:G:22:LEU:CG	3:G:26:LYS:HE3	1.91	1.00
1:y:354:PRO:HA	1:y:357:ARG:HG3	1.44	1.00
1:y:250:LYS:NZ	7:1:63:A:H4'	1.77	0.99
1:y:243:ARG:HB3	1:y:266:PRO:HB3	1.41	0.99
1:y:310:LEU:O	1:y:317:TYR:HB3	1.62	0.99
1:y:353:VAL:CG2	1:y:354:PRO:HD2	1.92	0.99
1:y:115:LYS:HD2	1:y:118:GLN:OE1	1.62	0.98
1:y:39:ILE:CG2	3:G:68:LEU:CD1	2.42	0.98
3:G:28:ALA:O	3:G:32:ALA:CB	2.12	0.98
2:E:126:ARG:NE	3:G:68:LEU:HD22	1.79	0.95
1:y:165:VAL:HG12	3:G:22:LEU:CD2	1.97	0.95
1:y:248:TYR:HD1	1:y:353:VAL:HA	1.30	0.95
2:E:126:ARG:HB3	3:G:68:LEU:HD21	0.95	0.95
1:y:267:LEU:HD13	1:y:268:LYS:H	1.29	0.94
3:G:55:MET:O	3:G:59:LEU:HG	1.65	0.94
3:G:62:LEU:O	3:G:66:ILE:HG13	1.69	0.93
1:y:248:TYR:CD1	1:y:353:VAL:HA	2.03	0.93
3:G:29:ASP:OD1	3:G:30:MET:N	2.03	0.92
1:y:169:MET:SD	3:G:22:LEU:O	2.28	0.91
3:G:28:ALA:O	3:G:32:ALA:HB2	1.70	0.91
1:y:365:TYR:OH	4:T:22:THR:HG21	1.71	0.90
1:y:169:MET:SD	3:G:22:LEU:HA	2.12	0.90
1:y:243:ARG:HB3	1:y:266:PRO:CB	2.01	0.88
1:y:267:LEU:CD1	1:y:268:LYS:H	1.86	0.87
1:y:251:ARG:CA	8:2:1336:A:OP1	2.23	0.87
2:E:126:ARG:NE	3:G:68:LEU:CD2	2.33	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:250:LYS:HZ1	7:1:63:A:H4'	1.36	0.86
1:y:122:TYR:O	1:y:125:LEU:HG	1.75	0.85
3:G:22:LEU:HG	3:G:26:LYS:HE3	1.57	0.85
3:G:22:LEU:CD1	3:G:26:LYS:HE3	2.05	0.85
3:G:47:GLY:O	3:G:48:SER:HB3	1.76	0.85
1:y:355:GLY:C	1:y:356:ILE:HG13	2.02	0.84
3:G:50:ASN:OD1	3:G:54:ARG:NH1	2.11	0.84
1:y:250:LYS:HB2	8:2:1336:A:H5'	1.60	0.83
1:y:39:ILE:HG21	3:G:68:LEU:CD1	2.07	0.83
3:G:18:GLY:HA2	3:G:63:PHE:CZ	2.14	0.82
3:G:22:LEU:HD11	3:G:26:LYS:HE3	1.62	0.81
1:y:353:VAL:HG22	1:y:354:PRO:CD	2.10	0.81
1:y:165:VAL:HG12	3:G:22:LEU:HD21	1.62	0.80
1:y:165:VAL:HG12	3:G:22:LEU:HD22	1.63	0.79
2:E:126:ARG:CZ	3:G:65:ILE:HG12	2.11	0.79
2:E:126:ARG:HH22	3:G:65:ILE:HG12	1.43	0.79
3:G:28:ALA:O	3:G:32:ALA:HB3	1.83	0.78
1:y:165:VAL:CG1	3:G:22:LEU:HD21	2.13	0.77
1:y:251:ARG:HA	8:2:1336:A:OP1	1.82	0.77
1:y:352:PHE:CE1	8:2:1318:U:C4'	2.66	0.77
1:y:250:LYS:HG3	4:T:68:LYS:HZ3	1.51	0.76
1:y:85:TYR:OH	3:G:38:ALA:HA	1.83	0.76
1:y:354:PRO:HG3	8:2:1337:G:O2'	1.84	0.76
3:G:53:THR:O	3:G:56:THR:OG1	2.03	0.75
1:y:115:LYS:CD	1:y:118:GLN:OE1	2.32	0.75
1:y:121:ARG:HD3	1:y:176:GLU:OE1	1.87	0.74
1:y:251:ARG:H	8:2:1336:A:P	2.10	0.74
1:y:165:VAL:CG1	3:G:22:LEU:CD2	2.65	0.74
1:y:338:ASN:H	1:y:339:PRO:CD	2.01	0.74
1:y:125:LEU:HD22	3:G:26:LYS:HD3	1.70	0.72
1:y:252:GLN:N	8:2:1336:A:OP1	2.22	0.72
3:G:73:ILE:HG22	3:G:73:ILE:O	1.88	0.71
1:y:248:TYR:CG	1:y:352:PHE:O	2.43	0.71
1:y:354:PRO:C	1:y:356:ILE:N	2.49	0.71
3:G:47:GLY:O	3:G:48:SER:CB	2.38	0.71
1:y:251:ARG:N	8:2:1336:A:OP1	2.25	0.70
1:y:354:PRO:CG	8:2:1337:G:O2'	2.39	0.70
1:y:354:PRO:CA	1:y:357:ARG:HG3	2.19	0.69
1:y:162:VAL:HG22	3:G:19:LEU:CD2	2.16	0.69
1:y:243:ARG:CB	1:y:266:PRO:HB3	2.21	0.69
1:y:39:ILE:HG22	3:G:68:LEU:HD13	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:354:PRO:O	1:y:355:GLY:C	2.36	0.69
1:y:115:LYS:NZ	1:y:118:GLN:OE1	2.25	0.69
1:y:172:MET:HE3	3:G:29:ASP:OD2	1.93	0.69
1:y:355:GLY:N	4:T:18:GLU:OE2	2.20	0.67
2:E:126:ARG:CG	3:G:68:LEU:HD21	2.24	0.67
1:y:166:THR:HA	3:G:22:LEU:HD13	1.75	0.67
1:y:338:ASN:H	1:y:339:PRO:HD3	1.60	0.66
3:G:62:LEU:O	3:G:66:ILE:CG1	2.43	0.66
1:y:169:MET:SD	3:G:22:LEU:CA	2.84	0.66
3:G:18:GLY:CA	3:G:63:PHE:CZ	2.78	0.65
1:y:172:MET:CE	3:G:29:ASP:OD2	2.44	0.65
1:y:354:PRO:HA	1:y:357:ARG:HG2	1.80	0.64
3:G:22:LEU:HD21	3:G:26:LYS:NZ	2.12	0.64
1:y:39:ILE:CG2	3:G:68:LEU:HD11	2.27	0.64
2:E:126:ARG:NH2	3:G:65:ILE:CG1	2.54	0.64
1:y:267:LEU:HD13	1:y:268:LYS:N	2.08	0.64
3:G:26:LYS:O	3:G:29:ASP:OD1	2.16	0.64
2:E:126:ARG:CG	3:G:68:LEU:CD2	2.76	0.63
1:y:170:PHE:CZ	3:G:61:THR:HG22	2.33	0.63
3:G:43:PHE:N	3:G:43:PHE:CD2	2.63	0.63
1:y:249:ALA:HA	8:2:1336:A:O2'	1.99	0.63
1:y:162:VAL:CG2	3:G:19:LEU:HD21	2.22	0.62
2:E:126:ARG:NH1	3:G:65:ILE:HG12	2.14	0.62
1:y:354:PRO:O	1:y:356:ILE:C	2.42	0.62
2:E:126:ARG:CB	3:G:68:LEU:CD2	2.63	0.62
1:y:169:MET:HB2	3:G:22:LEU:CD1	2.30	0.61
1:y:115:LYS:CE	1:y:118:GLN:OE1	2.48	0.61
1:y:354:PRO:C	1:y:356:ILE:H	2.08	0.61
1:y:114:ARG:NH1	3:G:34:PHE:CD1	2.69	0.61
1:y:349:SER:C	1:y:351:ALA:H	2.09	0.61
1:y:252:GLN:HE22	4:T:70:HIS:CD2	2.18	0.60
3:G:22:LEU:CD2	3:G:26:LYS:HE3	2.31	0.60
2:E:126:ARG:O	3:G:68:LEU:HD11	2.01	0.60
2:E:126:ARG:HE	3:G:68:LEU:HD23	1.56	0.59
3:G:43:PHE:N	3:G:43:PHE:HD2	1.99	0.59
1:y:250:LYS:HB2	8:2:1336:A:C5'	2.32	0.59
1:y:248:TYR:CD1	1:y:352:PHE:O	2.54	0.59
1:y:353:VAL:CG2	1:y:354:PRO:CD	2.74	0.59
1:y:85:TYR:OH	3:G:38:ALA:CB	2.51	0.59
1:y:365:TYR:HH	4:T:22:THR:HG21	1.64	0.59
1:y:122:TYR:HA	1:y:125:LEU:CD2	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:85:TYR:OH	3:G:38:ALA:CA	2.51	0.59
1:y:243:ARG:HB3	1:y:266:PRO:CA	2.32	0.58
1:y:255:ARG:N	7:1:91:A:N3	2.48	0.57
3:G:22:LEU:HD11	3:G:26:LYS:CE	2.34	0.57
1:y:169:MET:SD	3:G:22:LEU:C	2.86	0.57
1:y:250:LYS:HZ1	7:1:63:A:C4'	2.14	0.57
11:5:2162:G:H22	11:5:2164:C:H4'	1.69	0.57
3:G:65:ILE:O	3:G:68:LEU:HB3	2.04	0.57
1:y:248:TYR:HB2	1:y:352:PHE:O	2.05	0.56
1:y:125:LEU:HD12	1:y:126:VAL:N	2.21	0.56
3:G:43:PHE:HD2	3:G:43:PHE:H	1.53	0.56
3:G:21:MET:HE1	3:G:59:LEU:HB3	1.86	0.56
1:y:354:PRO:HA	1:y:357:ARG:CD	2.35	0.56
1:y:265:LEU:N	1:y:266:PRO:HD3	2.21	0.56
1:y:353:VAL:HG23	1:y:354:PRO:HD2	1.83	0.55
1:y:121:ARG:HH22	3:G:33:SER:HB3	1.72	0.55
3:G:17:VAL:HA	3:G:20:ILE:HD12	1.88	0.55
1:y:250:LYS:N	8:2:1336:A:H4'	2.21	0.55
3:G:63:PHE:HA	3:G:66:ILE:HD12	1.88	0.55
1:y:355:GLY:O	1:y:356:ILE:CB	2.54	0.54
4:T:3:ARG:HE	4:T:42:GLU:HG2	1.73	0.54
5:U:12:VAL:HG12	5:U:14:THR:H	1.72	0.54
1:y:417:MET:HB2	2:E:104:MET:HE2	1.89	0.54
1:y:169:MET:HB2	3:G:22:LEU:HD11	1.89	0.53
3:G:22:LEU:HD21	3:G:26:LYS:CE	2.38	0.53
1:y:245:VAL:C	1:y:246:VAL:HG23	2.34	0.53
1:y:274:VAL:HG13	1:y:411:VAL:CG1	2.38	0.53
2:E:126:ARG:NH2	3:G:65:ILE:HA	2.24	0.53
3:G:35:GLY:HA2	3:G:42:LEU:HD12	1.92	0.52
1:y:121:ARG:HD3	1:y:176:GLU:CD	2.33	0.52
1:y:169:MET:CB	3:G:22:LEU:CD1	2.88	0.52
3:G:22:LEU:HG	3:G:26:LYS:CE	2.37	0.52
1:y:250:LYS:HG3	4:T:68:LYS:NZ	2.22	0.52
1:y:39:ILE:HG23	3:G:68:LEU:HD11	1.91	0.52
1:y:250:LYS:H	8:2:1336:A:H4'	1.74	0.52
3:G:58:LEU:O	3:G:62:LEU:HG	2.11	0.51
1:y:248:TYR:CB	1:y:352:PHE:O	2.58	0.51
1:y:252:GLN:OE1	4:T:70:HIS:O	2.28	0.51
1:y:245:VAL:O	1:y:246:VAL:CG2	2.59	0.50
1:y:121:ARG:CD	1:y:176:GLU:OE1	2.59	0.50
1:y:354:PRO:C	1:y:357:ARG:HG3	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:250:LYS:HG3	4:T:68:LYS:HE2	1.93	0.50
4:T:4:GLU:H	4:T:7:LEU:HD23	1.76	0.50
1:y:310:LEU:O	1:y:311:GLN:O	2.30	0.50
1:y:354:PRO:O	1:y:356:ILE:CA	2.54	0.50
1:y:121:ARG:NH2	3:G:29:ASP:O	2.45	0.50
1:y:114:ARG:NH1	3:G:34:PHE:HD1	2.10	0.49
1:y:165:VAL:CG1	3:G:22:LEU:HD22	2.35	0.49
1:y:196:VAL:HG11	2:E:108:LEU:HB2	1.93	0.49
3:G:22:LEU:HD21	3:G:26:LYS:HE3	1.93	0.49
1:y:413:ILE:HD12	2:E:104:MET:HB3	1.93	0.49
1:y:253:GLN:C	7:1:91:A:N1	2.49	0.49
1:y:162:VAL:HG13	3:G:19:LEU:CD2	2.43	0.49
1:y:252:GLN:NE2	4:T:70:HIS:HD2	2.09	0.49
1:y:122:TYR:HD1	1:y:125:LEU:HD21	1.78	0.48
1:y:243:ARG:HB3	1:y:266:PRO:HA	1.94	0.48
1:y:252:GLN:NE2	4:T:70:HIS:CD2	2.81	0.48
1:y:354:PRO:CB	8:2:1337:G:O2'	2.61	0.48
3:G:55:MET:O	3:G:59:LEU:CG	2.52	0.48
4:T:58:VAL:HG22	4:T:85:VAL:HG13	1.94	0.48
1:y:292:SER:HA	1:y:304:THR:OG1	2.14	0.48
2:E:126:ARG:HH21	3:G:65:ILE:HA	1.78	0.48
1:y:169:MET:CB	3:G:22:LEU:HD12	2.43	0.47
1:y:250:LYS:HZ3	7:1:63:A:H4'	1.75	0.47
1:y:245:VAL:C	1:y:246:VAL:CG2	2.88	0.47
3:G:26:LYS:O	3:G:30:MET:HG3	2.15	0.47
10:4:1885:A:C8	10:4:1886:U:C5	3.03	0.47
1:y:162:VAL:HG13	3:G:19:LEU:HD23	1.96	0.47
11:5:2104:C:OP1	11:5:2104:C:H4'	2.14	0.46
3:G:58:LEU:O	3:G:62:LEU:CG	2.64	0.46
1:y:122:TYR:CD1	1:y:125:LEU:HD21	2.50	0.46
1:y:310:LEU:H	1:y:310:LEU:HG	1.61	0.46
11:5:2196:C:H2'	11:5:2197:U:C6	2.51	0.46
1:y:295:GLY:CA	1:y:300:TRP:O	2.64	0.46
10:4:1865:U:C5	10:4:1875:G:C6	3.04	0.45
1:y:413:ILE:HB	2:E:104:MET:HB3	1.98	0.45
1:y:265:LEU:HD21	1:y:342:THR:HG21	1.99	0.45
3:G:18:GLY:CA	3:G:63:PHE:HZ	2.28	0.45
1:y:250:LYS:HG3	4:T:68:LYS:CE	2.46	0.45
11:5:2128:G:C6	11:5:2160:C:C5	3.05	0.45
7:1:80:G:C2	7:1:107:G:C2	3.05	0.45
3:G:22:LEU:O	3:G:26:LYS:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:251:ARG:C	8:2:1336:A:OP1	2.60	0.45
1:y:349:SER:C	1:y:351:ALA:N	2.73	0.45
1:y:169:MET:CE	3:G:22:LEU:HA	2.47	0.44
1:y:227:VAL:HA	1:y:406:LEU:HD11	1.99	0.44
4:T:61:LEU:HD23	4:T:61:LEU:N	2.32	0.44
1:y:172:MET:HE1	3:G:29:ASP:OD2	2.18	0.44
2:E:95:LEU:HD12	2:E:95:LEU:H	1.82	0.44
1:y:39:ILE:HG22	3:G:68:LEU:CD1	2.38	0.44
1:y:180:GLU:CD	3:G:36:ALA:HB2	2.43	0.43
1:y:196:VAL:HG11	2:E:108:LEU:HD13	2.00	0.43
2:E:126:ARG:HG2	3:G:68:LEU:CD2	2.48	0.43
1:y:245:VAL:O	1:y:246:VAL:HG22	2.19	0.43
2:E:126:ARG:HH22	3:G:65:ILE:CG1	2.22	0.43
1:y:253:GLN:HB3	7:1:91:A:H61	1.83	0.43
1:y:264:HIS:ND1	1:y:264:HIS:N	2.68	0.42
1:y:355:GLY:C	1:y:356:ILE:CG1	2.75	0.42
3:G:21:MET:HE1	3:G:59:LEU:CB	2.48	0.42
3:G:29:ASP:HA	3:G:32:ALA:HB3	2.01	0.42
6:Y:60:LYS:HG3	6:Y:62:GLY:O	2.20	0.42
1:y:162:VAL:HA	3:G:19:LEU:HD21	2.02	0.42
3:G:35:GLY:HA2	3:G:42:LEU:CD1	2.50	0.42
10:4:1873:G:C6	10:4:1874:C:C4	3.08	0.42
1:y:122:TYR:O	1:y:125:LEU:CG	2.58	0.41
1:y:249:ALA:HA	8:2:1336:A:H4'	2.02	0.41
5:U:35:VAL:HB	5:U:38:ILE:HD11	2.02	0.41
6:Y:23:ARG:H	6:Y:26:PHE:HB3	1.85	0.41
5:U:1:ALA:HB3	5:U:84:PHE:CE1	2.55	0.41
1:y:354:PRO:HB2	4:T:18:GLU:OE2	2.20	0.41
5:U:32:LYS:HB3	5:U:63:ALA:HB1	2.03	0.41
2:E:126:ARG:NE	3:G:68:LEU:HD23	2.25	0.41
2:E:126:ARG:HG2	3:G:68:LEU:HD23	2.03	0.41
4:T:92:ASN:HD22	4:T:94:ASP:H	1.68	0.41
1:y:349:SER:O	1:y:351:ALA:N	2.54	0.40
1:y:125:LEU:HD12	1:y:126:VAL:HG23	2.02	0.40
1:y:357:ARG:NH1	8:2:1316:U:H1'	2.35	0.40
1:y:236:PHE:CD1	2:E:94:THR:HG21	2.57	0.40
6:Y:38:GLN:HE21	6:Y:43:LEU:CD1	2.34	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	y	435/437 (100%)	386 (89%)	27 (6%)	22 (5%)	1	15
2	E	54/56 (96%)	49 (91%)	3 (6%)	2 (4%)	2	20
3	G	63/65 (97%)	50 (79%)	7 (11%)	6 (10%)	0	8
4	T	98/100 (98%)	71 (72%)	18 (18%)	9 (9%)	0	8
5	U	101/103 (98%)	79 (78%)	13 (13%)	9 (9%)	0	8
6	Y	61/63 (97%)	48 (79%)	11 (18%)	2 (3%)	3	21
All	All	812/824 (98%)	683 (84%)	79 (10%)	50 (6%)	2	13

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	y	142	MET
1	y	258	TYR
1	y	266	PRO
1	y	338	ASN
1	y	340	ARG
1	y	355	GLY
1	y	356	ILE
3	G	44	GLY
3	G	48	SER
3	G	51	PHE
5	U	49	PRO
1	y	215	LEU
1	y	270	ASN
1	y	354	PRO
1	y	394	ALA
3	G	45	SER
3	G	52	MET
4	T	10	VAL
4	T	21	SER
5	U	12	VAL

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Mol	Chain	Res	Type
5	U	47	PRO
1	y	313	GLY
2	E	89	GLU
2	E	125	LEU
3	G	35	GLY
4	T	18	GLU
4	T	52	GLU
4	T	86	THR
5	U	73	ASN
5	U	80	ASP
6	Y	2	LYS
6	Y	37	LEU
1	y	183	ILE
1	y	311	GLN
1	y	396	LYS
4	T	36	LYS
5	U	7	ASP
5	U	81	ARG
1	y	214	ASP
1	y	255	ARG
1	y	269	VAL
4	T	38	ALA
4	T	76	ARG
5	U	5	ARG
5	U	74	ALA
1	y	256	ARG
1	y	350	GLY
1	y	246	VAL
4	T	74	ILE
1	y	274	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	y	353/353 (100%)	335 (95%)	18 (5%)	21 42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	47/47 (100%)	44 (94%)	3 (6%)	16	37
3	G	46/46 (100%)	43 (94%)	3 (6%)	15	37
4	T	84/84 (100%)	79 (94%)	5 (6%)	17	39
5	U	84/84 (100%)	80 (95%)	4 (5%)	23	44
6	Y	55/55 (100%)	53 (96%)	2 (4%)	31	52
All	All	669/669 (100%)	634 (95%)	35 (5%)	22	42

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	y	13	LYS
1	y	77	ILE
1	y	149	VAL
1	y	174	LEU
1	y	223	VAL
1	y	244	ILE
1	y	264	HIS
1	y	265	LEU
1	y	267	LEU
1	y	268	LYS
1	y	269	VAL
1	y	289	THR
1	y	298	THR
1	y	310	LEU
1	y	312	PRO
1	y	349	SER
1	y	397	VAL
1	y	409	VAL
2	E	76	ARG
2	E	90	THR
2	E	103	VAL
3	G	43	PHE
3	G	45	SER
3	G	46	SER
4	T	9	LYS
4	T	10	VAL
4	T	39	THR
4	T	61	LEU
4	T	73	ARG
5	U	4	ILE

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Mol	Chain	Res	Type
5	U	23	LYS
5	U	35	VAL
5	U	49	PRO
6	Y	30	MET
6	Y	46	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	y	10	GLN
1	y	56	GLN
1	y	141	ASN
1	y	146	GLN
1	y	241	GLN
1	y	252	GLN
1	y	270	ASN
4	T	59	ASN
4	T	70	HIS
4	T	91	GLN
4	T	92	ASN
5	U	65	GLN
6	Y	27	ASN
6	Y	36	GLN
6	Y	41	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	4	60/61 (98%)	2 (3%)	0
11	5	107/108 (99%)	37 (34%)	8 (7%)
7	1	62/63 (98%)	12 (19%)	0
8	2	35/36 (97%)	9 (25%)	2 (5%)
9	3	17/18 (94%)	5 (29%)	0
All	All	281/286 (98%)	65 (23%)	10 (3%)

All (65) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	1	63	A
7	1	64	A

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Mol	Chain	Res	Type
7	1	71	A
7	1	74	A
7	1	75	G
7	1	84	A
7	1	90	U
7	1	92	U
7	1	95	A
7	1	100	U
7	1	102	U
7	1	103	A
8	2	1312	U
8	2	1313	U
8	2	1316	U
8	2	1325	U
8	2	1326	U
8	2	1332	G
8	2	1333	G
8	2	1334	G
8	2	1336	A
9	3	1532	A
9	3	1535	A
9	3	1536	C
9	3	1538	G
9	3	1540	G
10	4	1870	C
10	4	1896	G
11	5	2102	G
11	5	2104	C
11	5	2111	U
11	5	2116	G
11	5	2117	A
11	5	2118	U
11	5	2119	A
11	5	2120	G
11	5	2121	G
11	5	2126	A
11	5	2127	G
11	5	2128	G
11	5	2130	U
11	5	2132	U
11	5	2135	A
11	5	2136	G

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Mol	Chain	Res	Type
11	5	2137	U
11	5	2145	C
11	5	2146	C
11	5	2147	A
11	5	2148	G
11	5	2149	U
11	5	2153	C
11	5	2155	U
11	5	2158	A
11	5	2160	C
11	5	2163	A
11	5	2164	C
11	5	2165	C
11	5	2166	U
11	5	2167	U
11	5	2176	A
11	5	2179	C
11	5	2181	U
11	5	2192	U
11	5	2198	A
11	5	2199	A

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	2	1312	U
8	2	1332	G
11	5	2116	G
11	5	2120	G
11	5	2126	A
11	5	2144	G
11	5	2145	C
11	5	2152	G
11	5	2164	C
11	5	2172	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

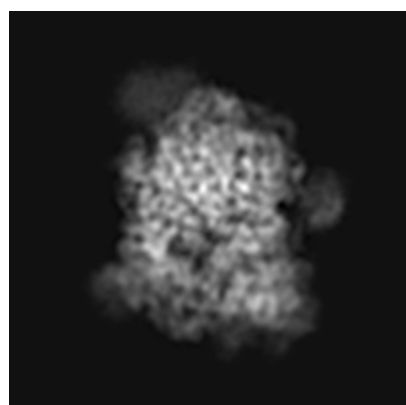
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5692. These allow visual inspection of the internal detail of the map and identification of artifacts.

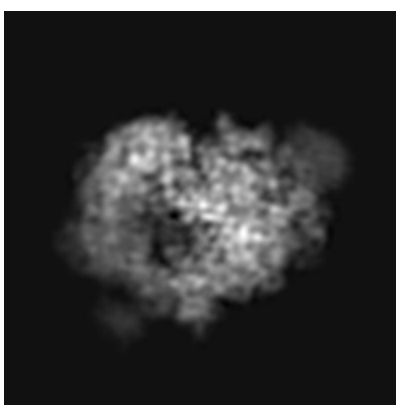
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

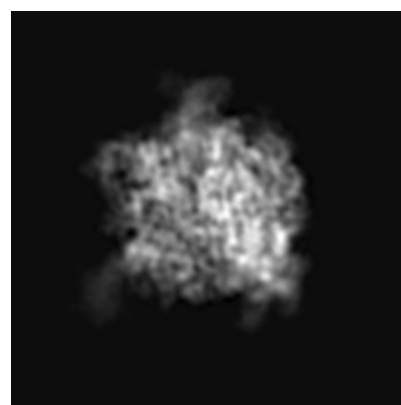
6.1.1 Primary map



X



Y

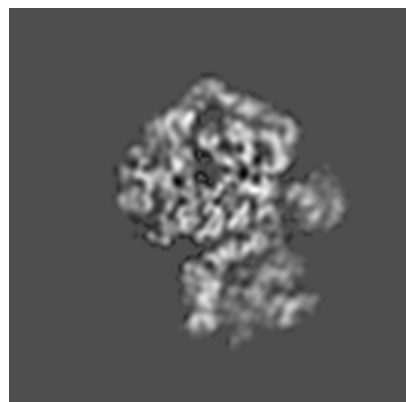


Z

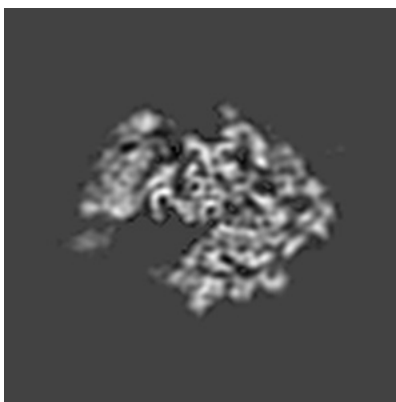
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

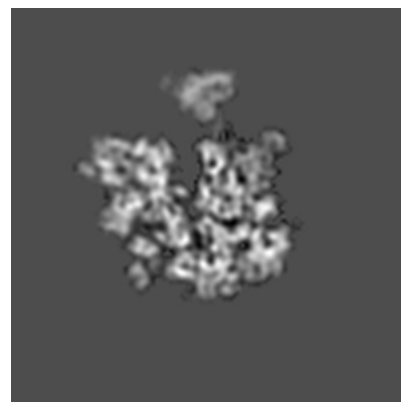
6.2.1 Primary map



X Index: 72



Y Index: 72

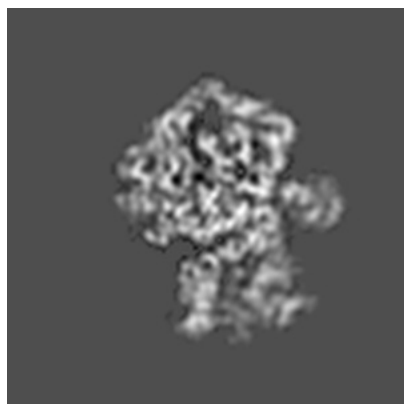


Z Index: 72

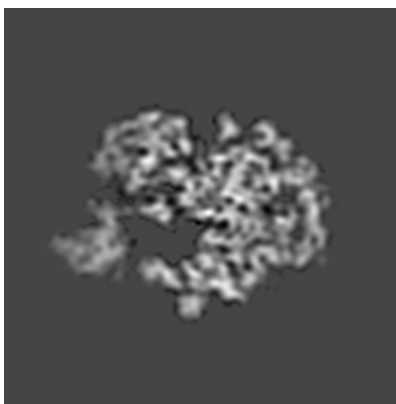
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

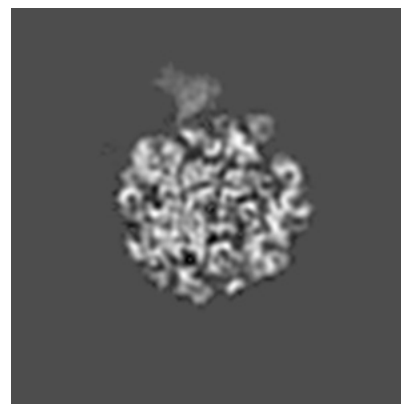
6.3.1 Primary map



X Index: 73



Y Index: 77

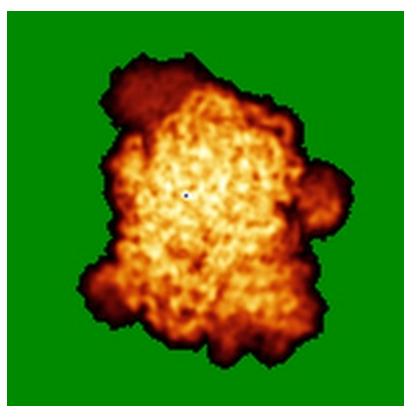


Z Index: 81

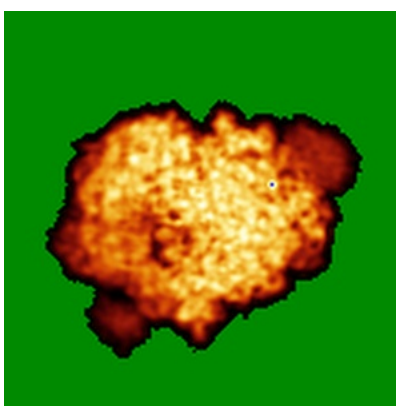
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X



Y

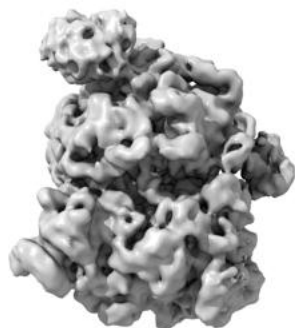


Z

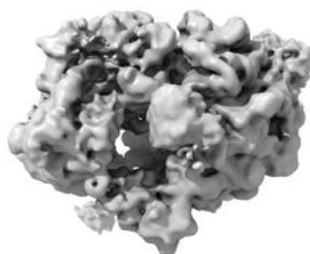
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

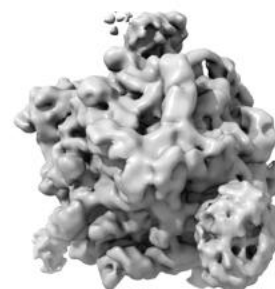
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

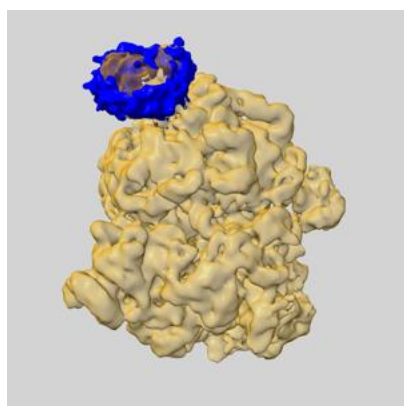
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

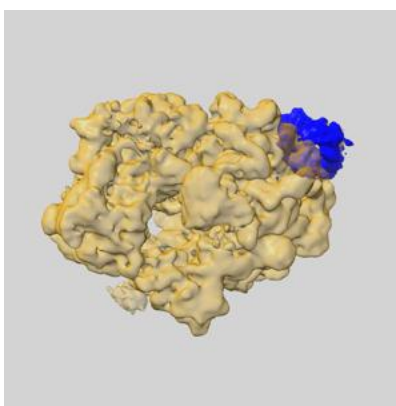
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

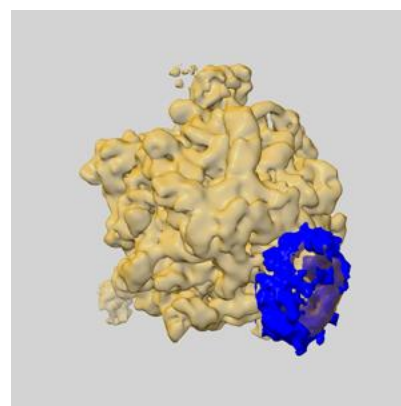
6.6.1 emd_5692_msk_4.map [i](#)



X

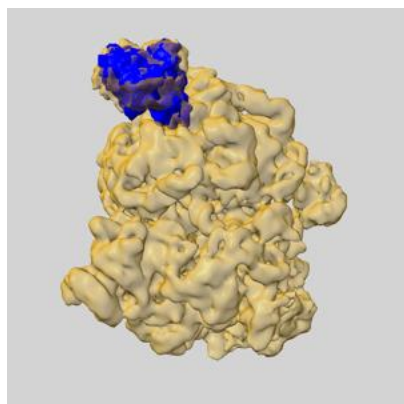


Y

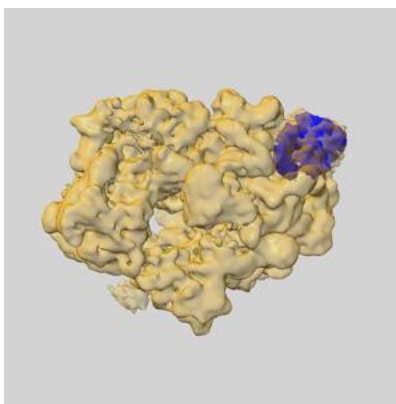


Z

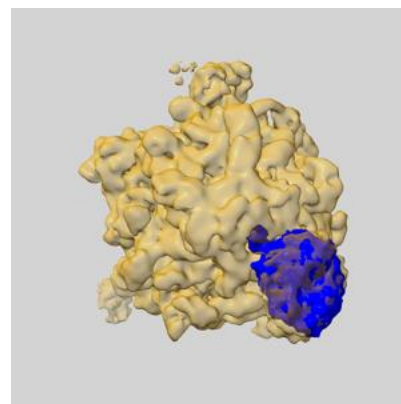
6.6.2 emd_5692_msk_3.map [i](#)



X

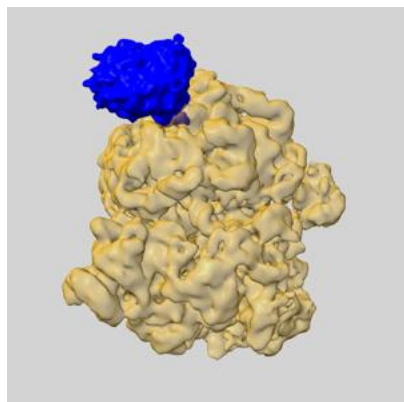


Y

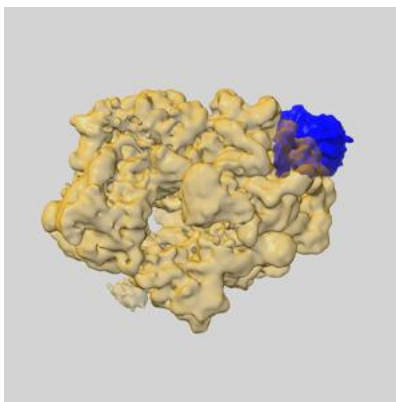


Z

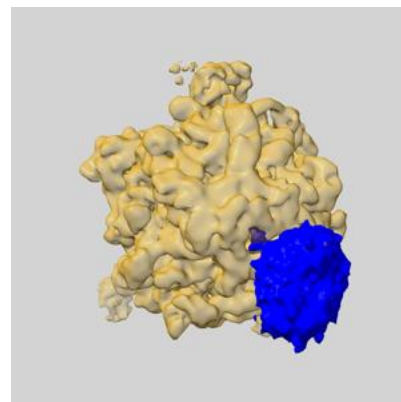
6.6.3 emd_5692_msk_2.map [i](#)



X

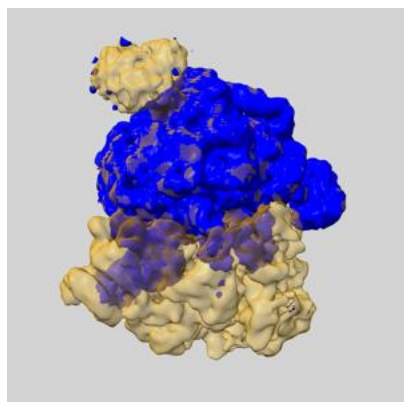


Y

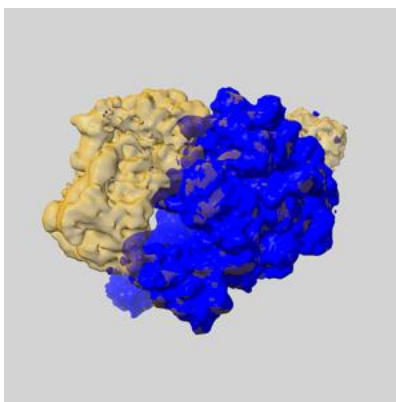


Z

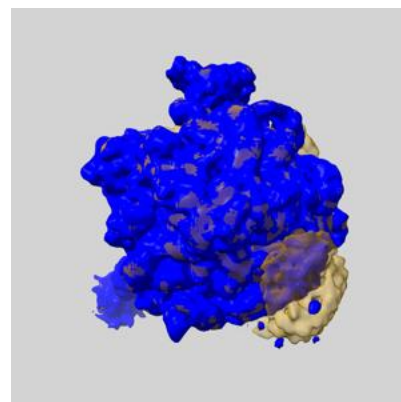
6.6.4 emd_5692_msk_1.map [i](#)



X

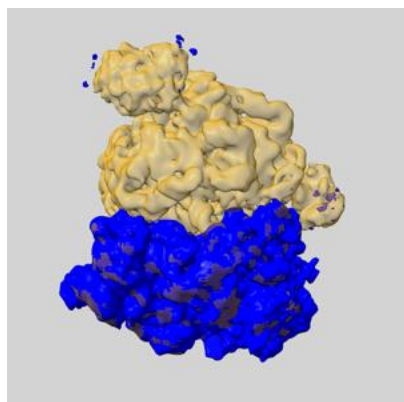


Y

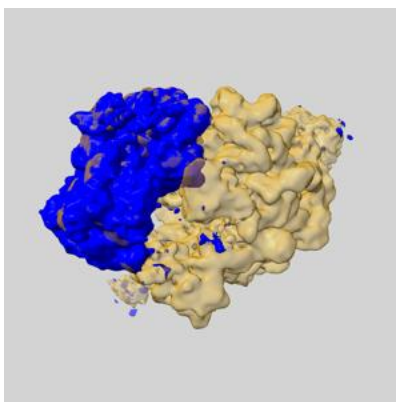


Z

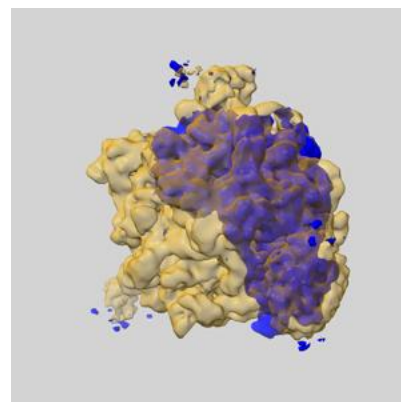
6.6.5 emd_5692_msk_5.map [i](#)



X



Y

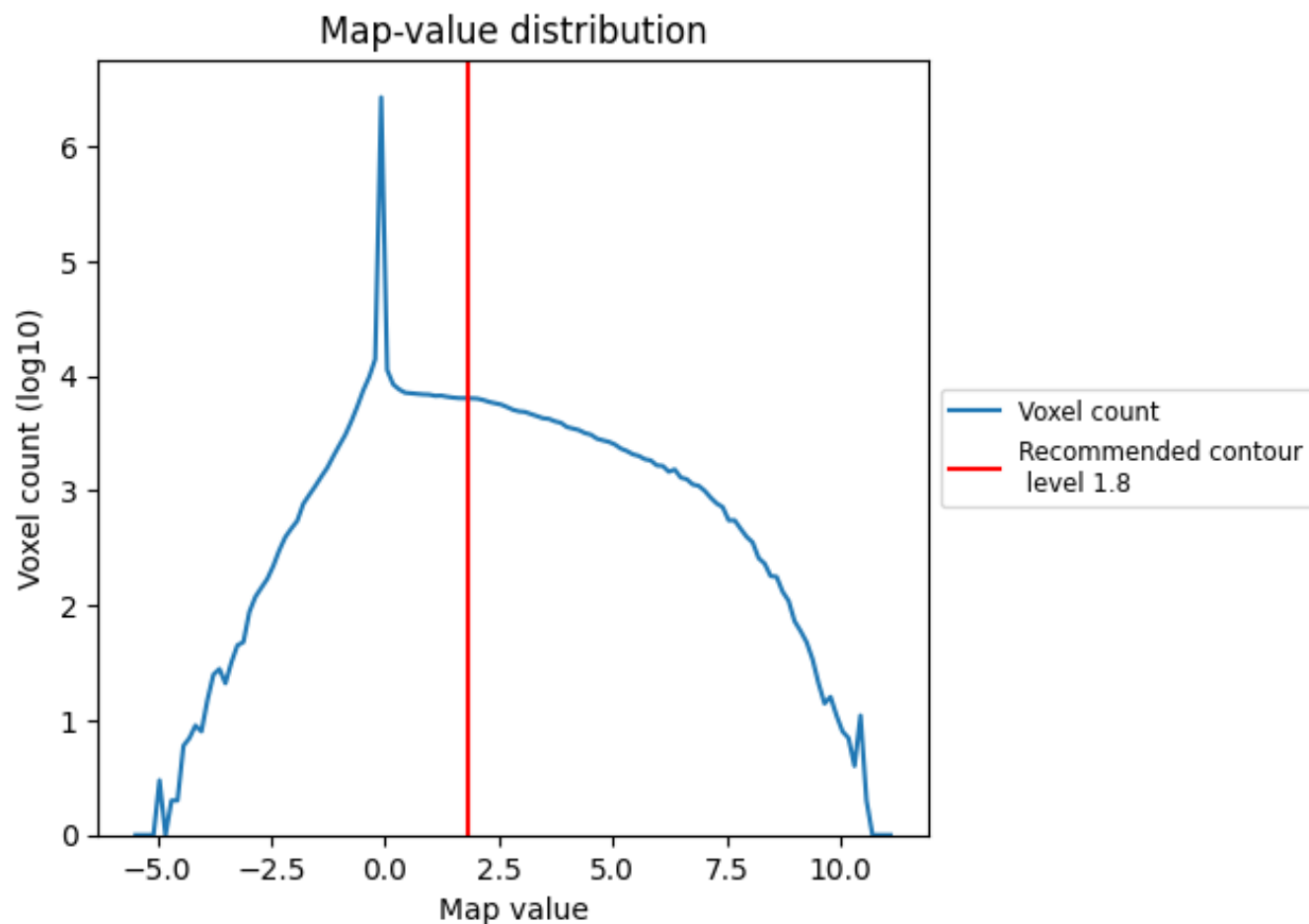


Z

7 Map analysis [i](#)

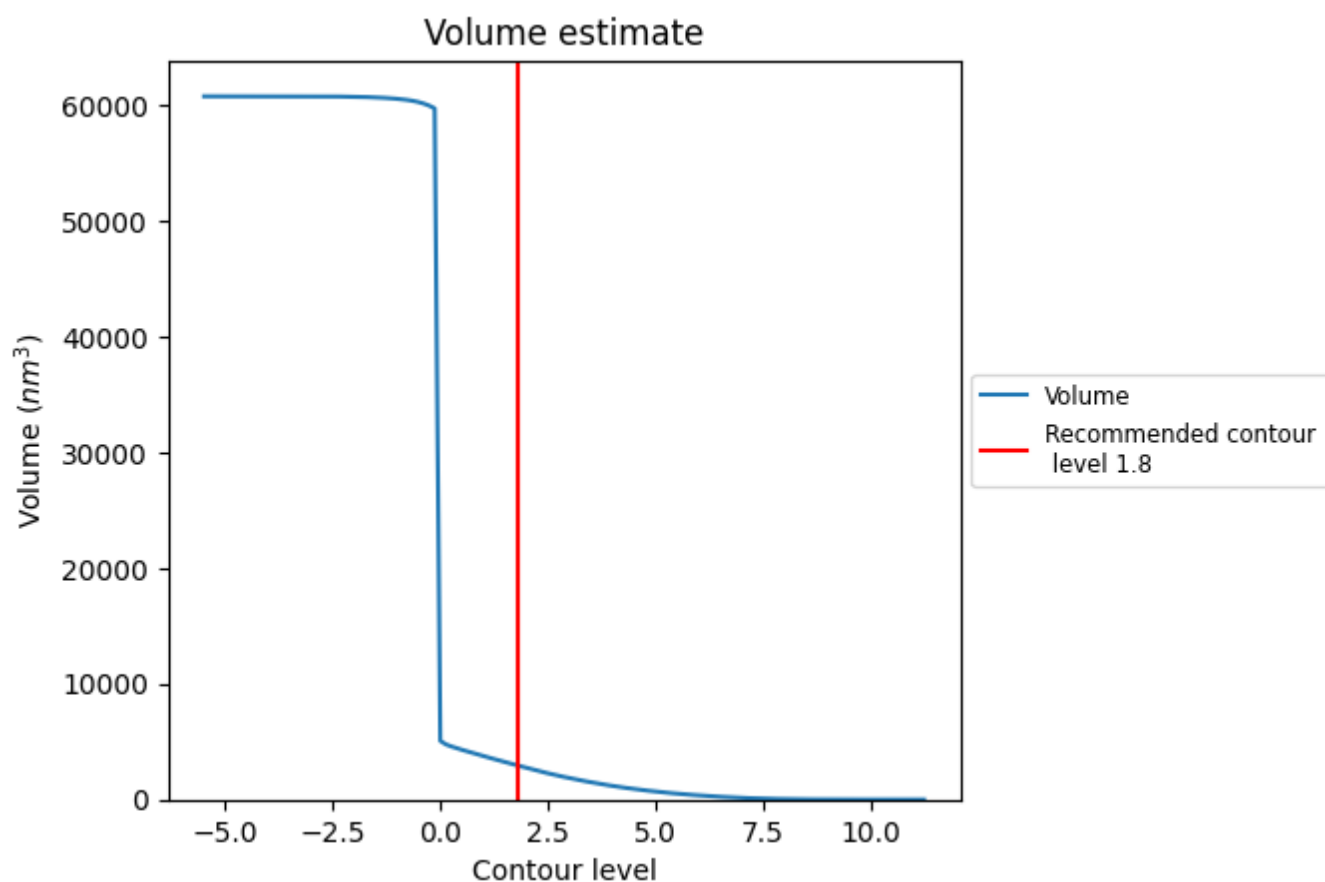
This section contains the results of statistical analysis of the map.

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.

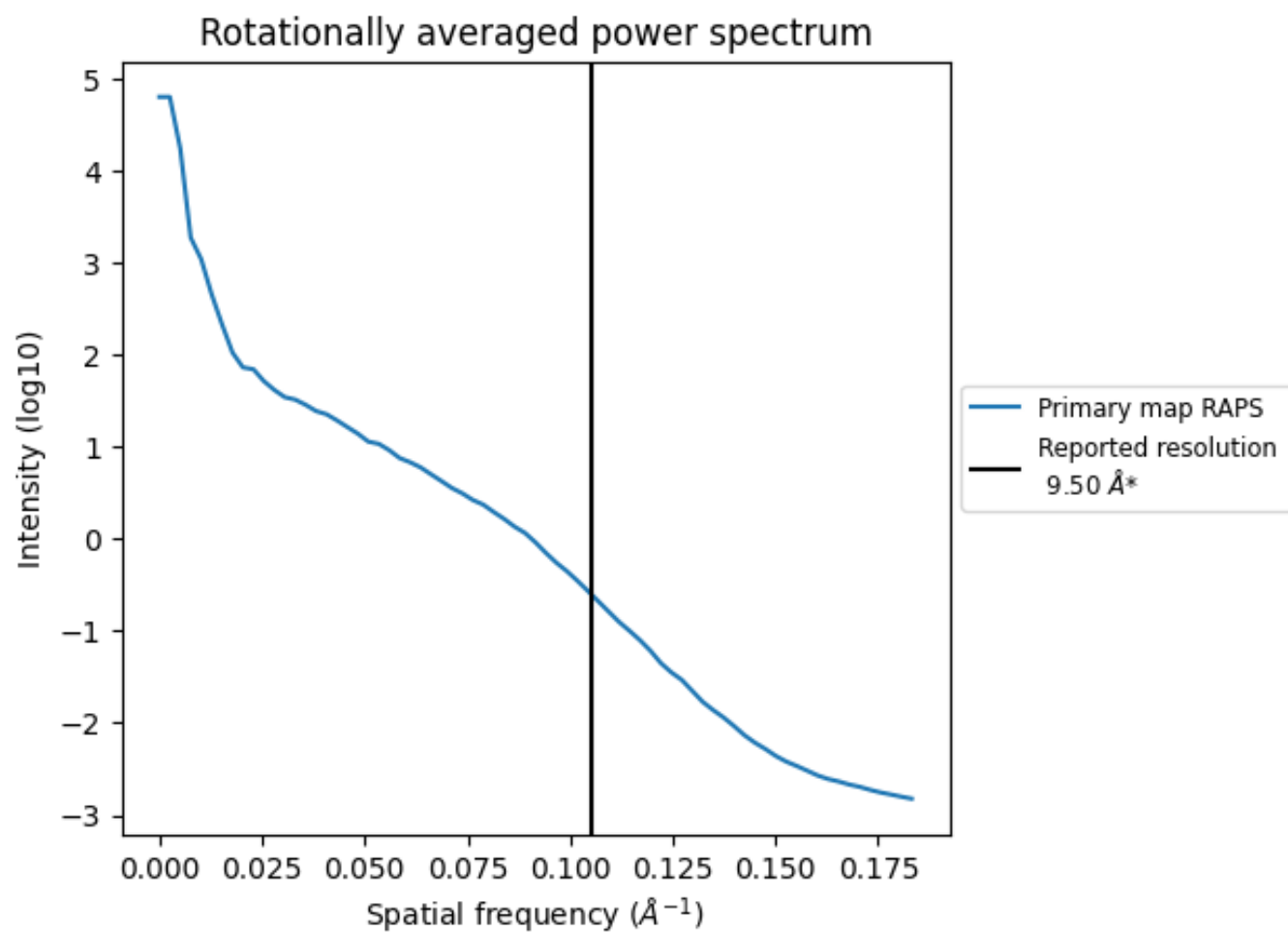
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2943 nm³; this corresponds to an approximate mass of 2659 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.105 Å⁻¹

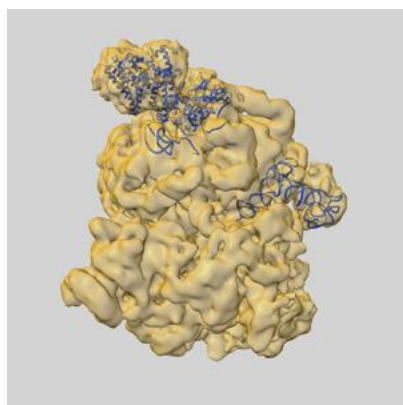
8 Fourier-Shell correlation ⓘ

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

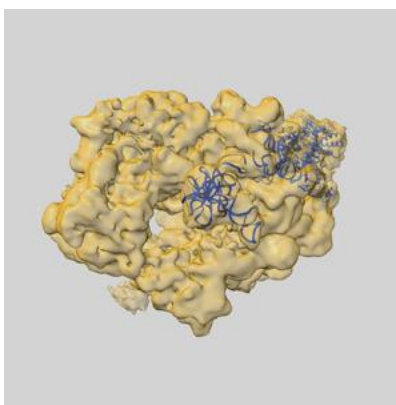
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-5692 and PDB model 3J45. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

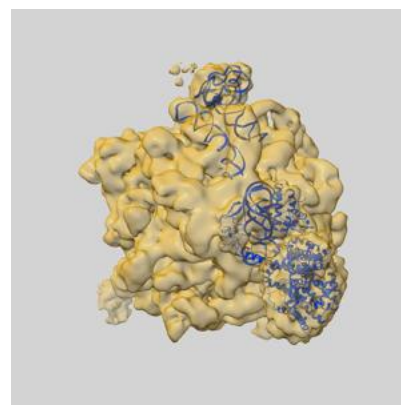
9.1 Map-model overlay [i](#)



X



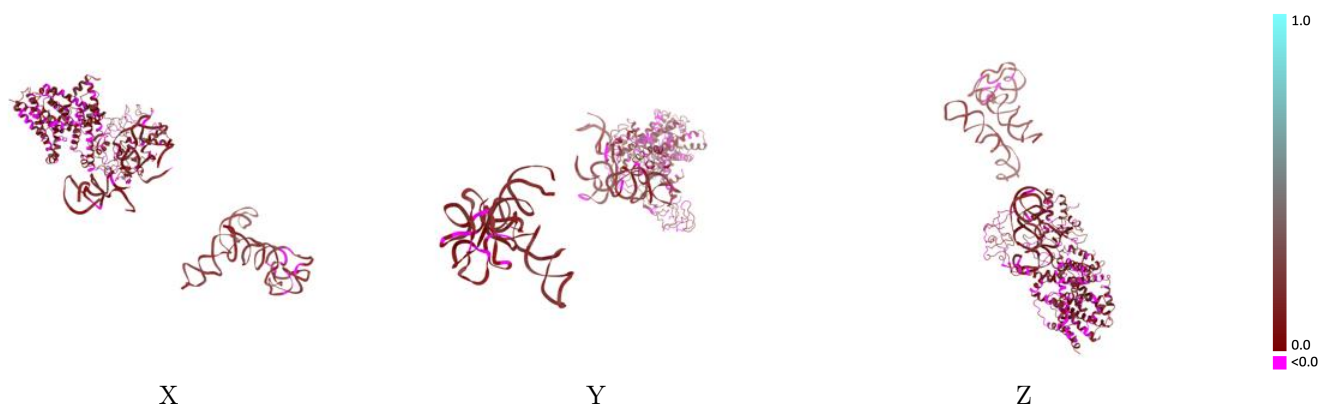
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.8 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](#)

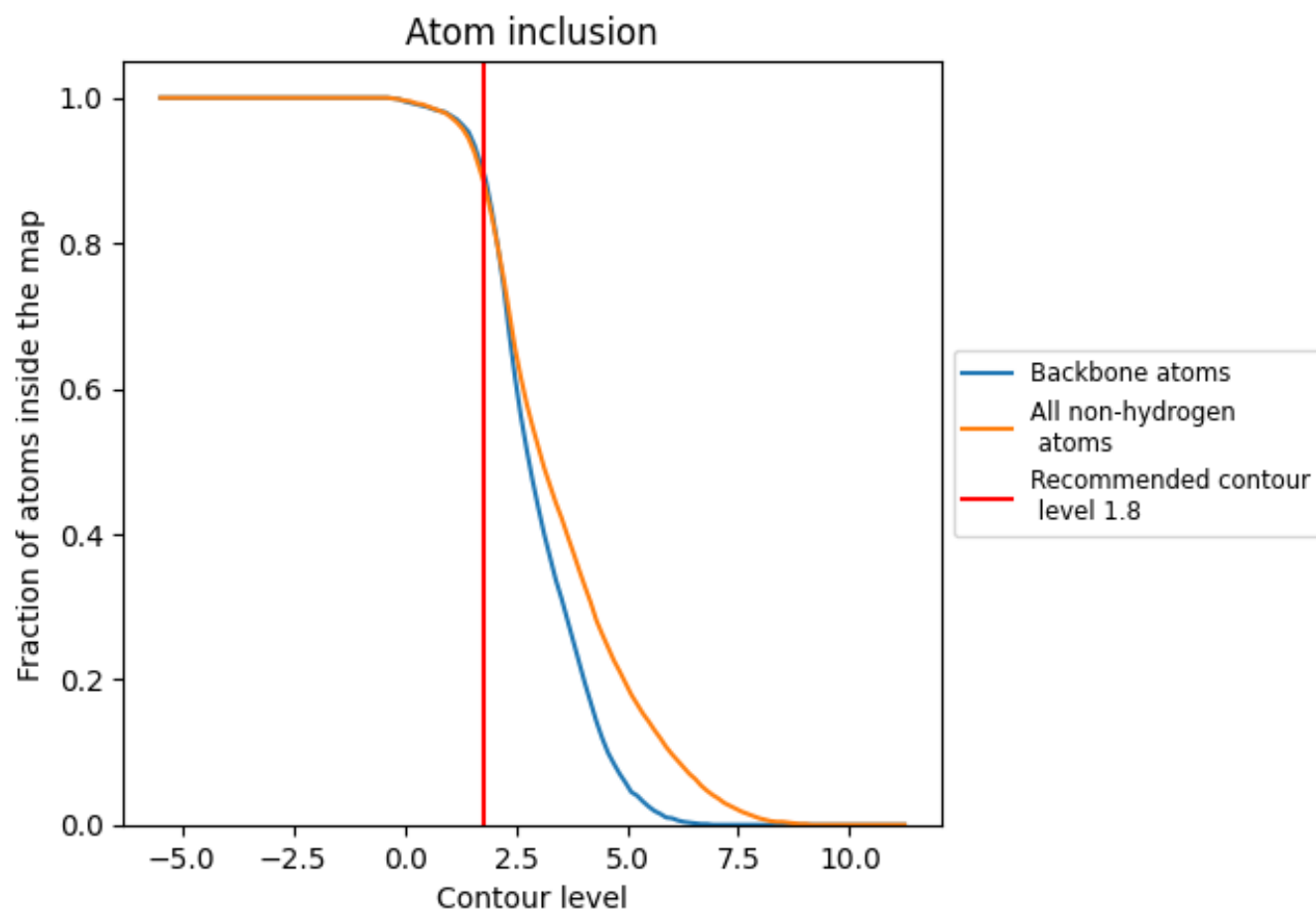


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (1.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8800	0.1030
1	0.9840	0.1370
2	0.9830	0.1250
3	0.9480	0.1510
4	0.9780	0.1660
5	0.9560	0.1170
E	0.7570	0.0690
G	0.7140	0.0290
T	0.8370	0.0830
U	0.8850	0.0870
Y	0.9280	0.1180
y	0.7550	0.0660

1.0
0.0
<0.0