



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 04:33 PM UTC

PDB ID : 3J5S / pdb_00003j5s
EMDB ID : EMD-5784
Title : EttA binds to ribosome exit site and regulates translation by restricting ribosome and tRNA dynamics
Authors : Hashem, Y.
Deposited on : 2013-11-15
Resolution : 7.50 Å (reported)
Based on initial models : 3R8O, 2WDG, 4FIN, 3R8T

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
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

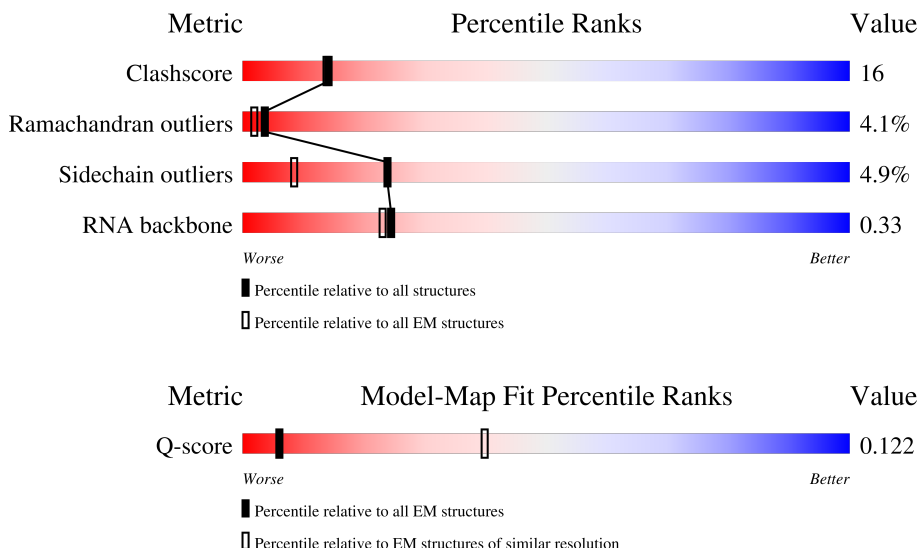
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.50 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	436 (7.00 - 8.00)

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	B	101	
2	A	360	
3	E	77	

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Mol	Chain	Length	Quality of chain
4	D	561	18% 44% 43% 12% ••
5	F	234	5% 39% 48% 12% •
6	G	178	6% 49% 43% 7% •
7	H	50	12% 52% 34% 14%
8	I	151	23% 42% 42% 15% •

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 15196 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	32	Total	C	N	O	P	0	0
			687	306	126	223	32		

- Molecule 2 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	174	Total	C	N	O	P	0	0
			3731	1663	674	1220	174		

- Molecule 3 is a RNA chain called P-site tRNA FMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

- Molecule 4 is a protein called Energy-dependent translational throttle A (EttA).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	554	Total	C	N	O	S	0	0
			4393	2764	781	837	11		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	HIS	-	expression tag	UNP P0A9W3
D	-4	HIS	-	expression tag	UNP P0A9W3
D	-3	HIS	-	expression tag	UNP P0A9W3
D	-2	HIS	-	expression tag	UNP P0A9W3
D	-1	HIS	-	expression tag	UNP P0A9W3
D	0	HIS	-	expression tag	UNP P0A9W3

- Molecule 5 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	234	Total	C	N	O	S	0	0
			1733	1081	315	330	7		

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	178	Total	C	N	O	S	0	0
			1420	905	251	258	6		

- Molecule 7 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	H	50	Total	C	N	O	0	0
			410	263	75	72		

- Molecule 8 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	151	Total	C	N	O	S	0	0
			1182	735	227	216	4		

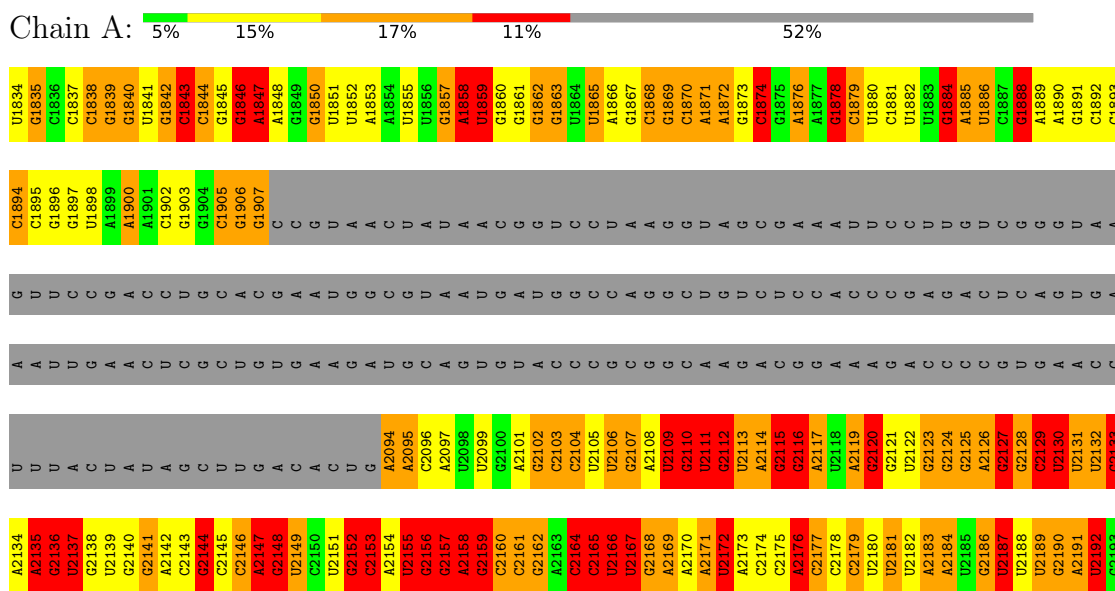
3 Residue-property plots

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.

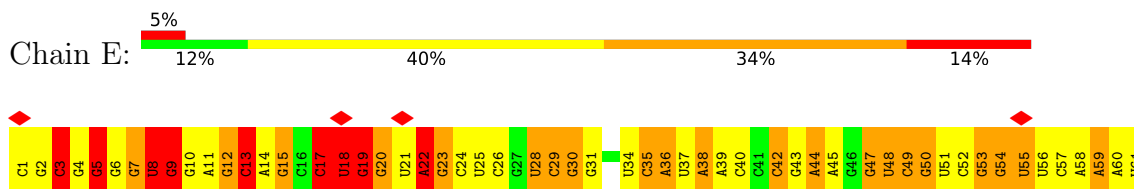
• Molecule 1: 16S ribosomal RNA



• Molecule 2: 23S ribosomal RNA

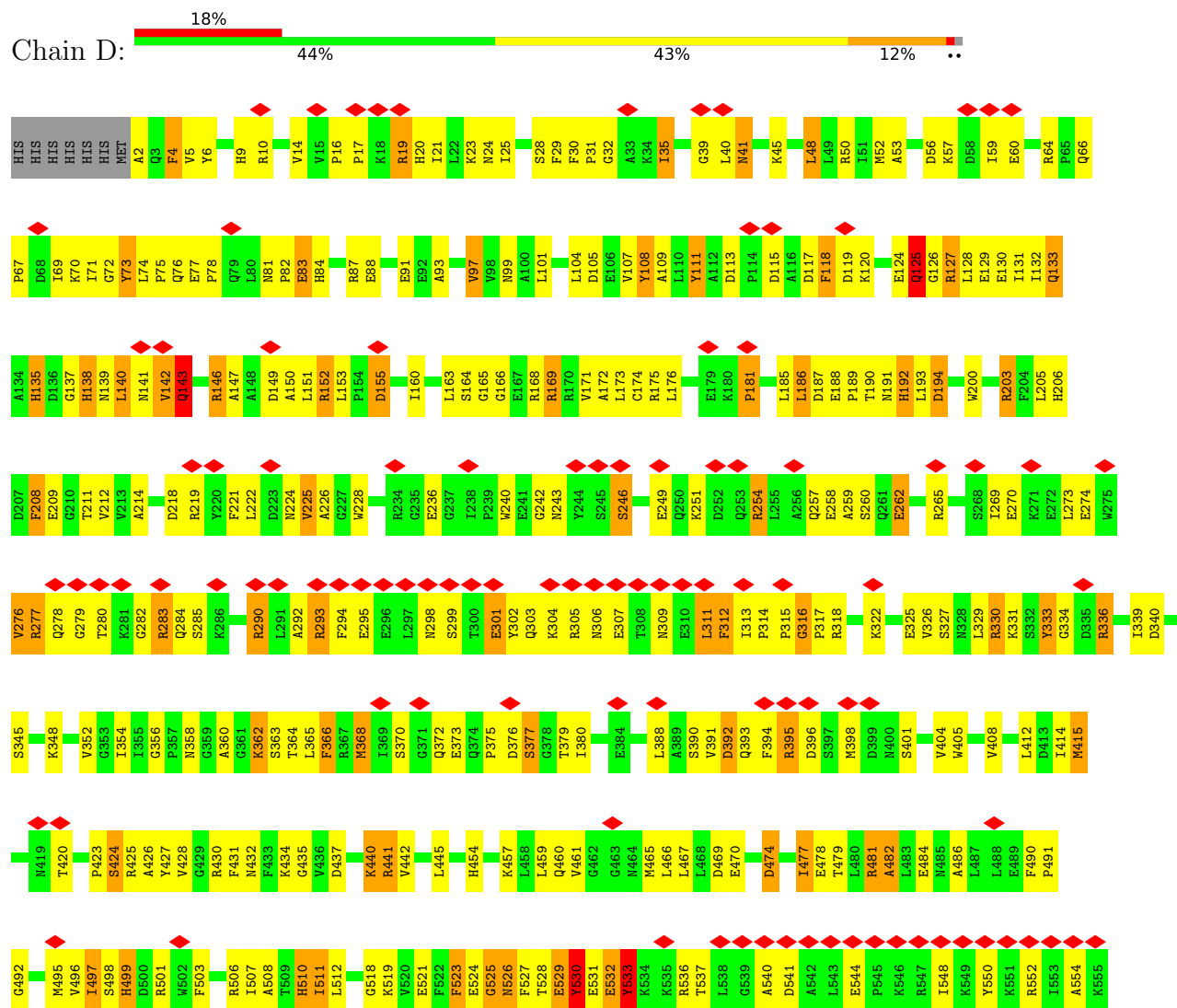


• Molecule 3: P-site tRNA FMet

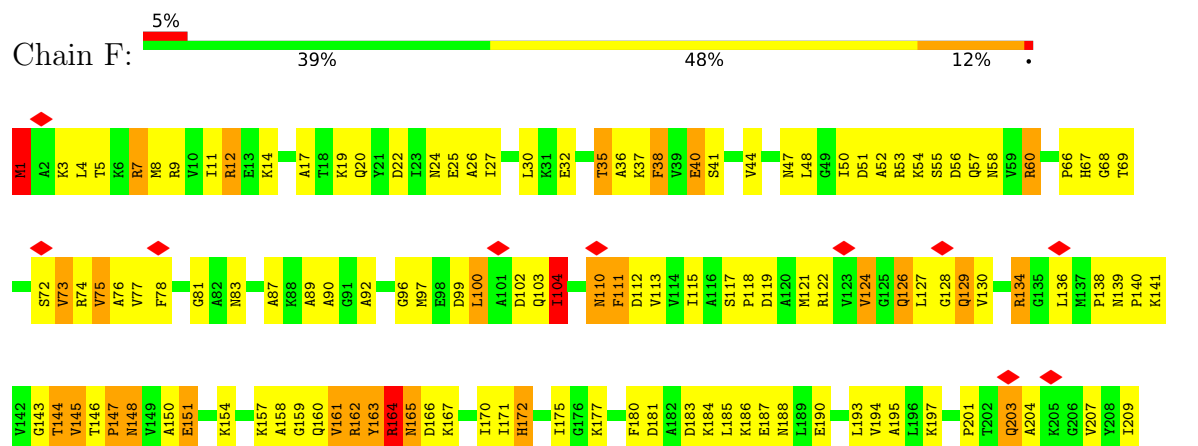


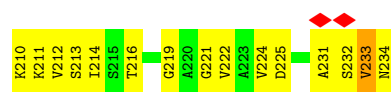


• Molecule 4: Energy-dependent translational throttle A (EttA)

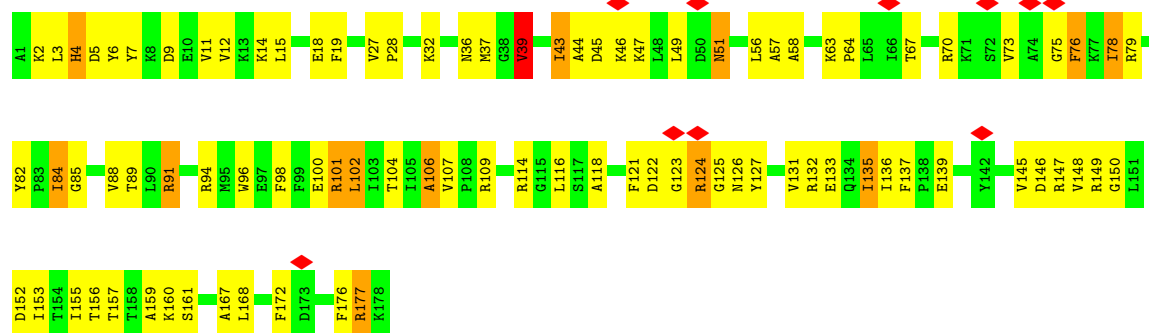


• Molecule 5: 50S ribosomal protein L1

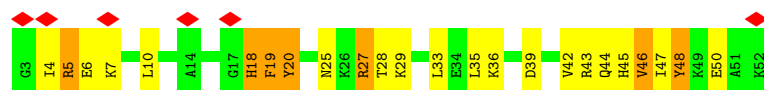




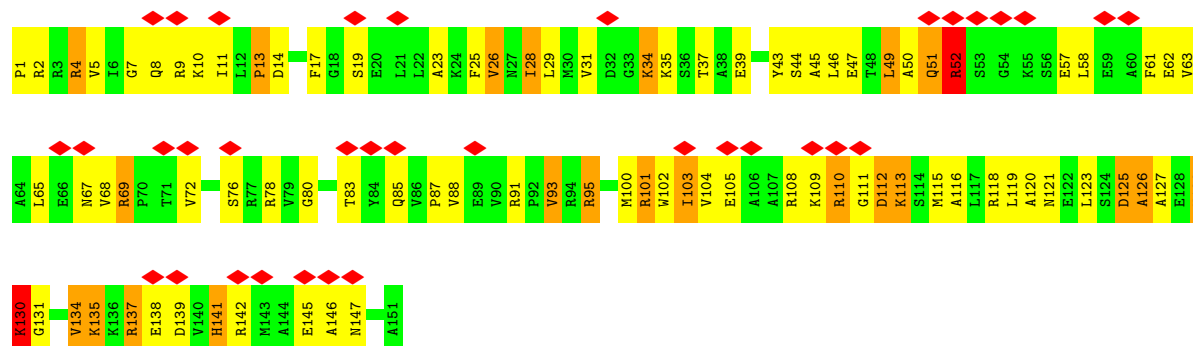
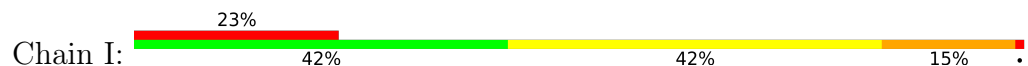
• Molecule 6: 50S ribosomal protein L5



• Molecule 7: 50S ribosomal protein L33



• Molecule 8: 30S ribosomal protein S7



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	39316	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Each micrograph	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	17	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	110637	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum map value	338.729	Depositor
Minimum map value	-150.118	Depositor
Average map value	3.621	Depositor
Map value standard deviation	39.948	Depositor
Recommended contour level	80	Depositor
Map size ($\text{\AA}$)	363.3544, 363.3544, 363.3544	wwPDB
Map dimensions	134, 134, 134	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	2.7116, 2.7116, 2.7116	Depositor

5 Model quality

5.1 Standard geometry

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	B	2.01	19/766 (2.5%)	1.82	27/1188 (2.3%)
2	A	2.03	106/4174 (2.5%)	1.80	130/6507 (2.0%)
3	E	2.03	40/1832 (2.2%)	1.77	50/2855 (1.8%)
4	D	2.10	110/4474 (2.5%)	2.46	302/6034 (5.0%)
5	F	2.10	52/1748 (3.0%)	2.54	135/2355 (5.7%)
6	G	2.16	37/1444 (2.6%)	2.44	90/1937 (4.6%)
7	H	2.21	14/417 (3.4%)	2.46	20/554 (3.6%)
8	I	2.11	28/1196 (2.3%)	2.51	87/1602 (5.4%)
All	All	2.08	406/16051 (2.5%)	2.19	841/23032 (3.7%)

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	B	0	12
2	A	0	84
3	E	0	34
4	D	0	23
5	F	0	9
6	G	0	6
7	H	0	4
8	I	0	6
All	All	0	178

All (406) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	510	HIS	ND1-CE1	11.30	1.43	1.32
4	D	16	PRO	CA-C	10.09	1.61	1.52
7	H	46	VAL	CA-CB	-9.29	1.48	1.55
6	G	114	ARG	C-O	-9.21	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	56	ASP	CA-CB	8.77	1.65	1.53
2	A	1837	C	C1'-N1	8.65	1.61	1.48
4	D	334	GLY	CA-C	-8.58	1.39	1.51
4	D	24	ASN	C-N	8.56	1.42	1.33
2	A	1886	U	C5'-C4'	8.41	1.63	1.51
5	F	32	GLU	CA-CB	8.34	1.67	1.53
6	G	131	VAL	C-N	8.29	1.45	1.33
4	D	35	ILE	CA-CB	-8.29	1.44	1.54
3	E	20	G	C4'-O4'	-8.24	1.33	1.45
4	D	120	LYS	CA-C	8.20	1.64	1.52
7	H	45	HIS	C-N	8.20	1.38	1.33
6	G	160	LYS	N-CA	-8.15	1.36	1.46
4	D	313	ILE	CA-CB	-8.10	1.48	1.54
4	D	441	ARG	CD-NE	8.09	1.57	1.46
7	H	48	TYR	N-CA	-8.00	1.36	1.45
2	A	2175	C	O5'-C5'	7.97	1.54	1.42
4	D	242	GLY	CA-C	-7.96	1.43	1.52
4	D	331	LYS	C-N	7.94	1.44	1.33
2	A	2115	G	C5'-C4'	7.93	1.63	1.51
2	A	2161	C	C5'-C4'	7.78	1.62	1.51
2	A	2158	A	C5'-C4'	7.76	1.62	1.51
6	G	98	PHE	CA-CB	7.67	1.65	1.53
4	D	132	ILE	CA-CB	-7.62	1.45	1.54
3	E	47	G	C3'-O3'	7.57	1.53	1.42
8	I	25	PHE	CA-C	7.55	1.62	1.52
2	A	2173	A	O3'-P	-7.54	1.49	1.61
2	A	2166	U	C5'-C4'	7.51	1.62	1.51
2	A	2111	U	C5'-C4'	7.50	1.62	1.51
2	A	2122	U	O3'-P	-7.48	1.50	1.61
1	B	1239	A	O3'-P	-7.42	1.50	1.61
8	I	7	GLY	N-CA	7.42	1.51	1.44
3	E	35	C	O3'-P	-7.40	1.50	1.61
4	D	206	HIS	ND1-CE1	7.36	1.40	1.32
8	I	93	VAL	CA-CB	7.35	1.62	1.54
2	A	1839	G	O4'-C1'	7.34	1.52	1.41
4	D	521	GLU	N-CA	-7.34	1.37	1.46
2	A	1847	A	O3'-P	-7.30	1.50	1.61
2	A	2112	G	C5'-C4'	7.30	1.62	1.51
8	I	2	ARG	CD-NE	7.30	1.56	1.46
2	A	1838	C	C5'-C4'	7.29	1.62	1.51
2	A	2167	U	C4'-O4'	7.24	1.56	1.45
4	D	260	SER	CA-C	7.21	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2110	G	C4'-C3'	7.20	1.64	1.53
4	D	548	ILE	N-CA	-7.19	1.38	1.46
8	I	4	ARG	CD-NE	7.18	1.56	1.46
4	D	193	LEU	CA-CB	7.17	1.64	1.53
3	E	48	U	O3'-P	-7.16	1.50	1.61
2	A	2115	G	P-O5'	-7.16	1.49	1.59
3	E	55	U	P-O5'	-7.13	1.49	1.59
3	E	26	C	O3'-P	7.12	1.71	1.61
4	D	437	ASP	C-N	7.12	1.43	1.34
4	D	88	GLU	N-CA	7.12	1.55	1.46
8	I	65	LEU	CA-CB	7.12	1.64	1.53
2	A	2158	A	O3'-P	-7.11	1.50	1.61
4	D	425	ARG	CA-C	-7.09	1.43	1.52
3	E	24	C	C5'-C4'	7.08	1.61	1.51
4	D	525	GLY	C-N	7.05	1.42	1.33
7	H	27	ARG	CD-NE	7.05	1.56	1.46
2	A	2146	C	C5'-C4'	7.00	1.61	1.51
3	E	69	C	C5'-C4'	7.00	1.61	1.51
2	A	2099	U	C3'-O3'	7.00	1.52	1.42
4	D	143	GLN	N-CA	6.98	1.55	1.46
2	A	2189	U	C3'-O3'	6.97	1.52	1.42
1	B	1305	G	C2'-C1'	-6.96	1.43	1.53
1	B	1290	G	C4'-C3'	6.95	1.62	1.52
4	D	316	GLY	N-CA	6.94	1.54	1.44
3	E	75	C	C4'-C3'	6.93	1.62	1.52
1	B	1298	U	C2'-C1'	-6.90	1.42	1.53
3	E	77	A	C4'-O4'	-6.90	1.35	1.45
2	A	1852	U	O3'-P	-6.86	1.50	1.61
2	A	2142	A	O3'-P	-6.86	1.50	1.61
8	I	100	MET	CA-CB	6.79	1.63	1.53
2	A	1867	G	O3'-P	-6.78	1.50	1.61
7	H	33	LEU	CA-CB	6.75	1.64	1.53
2	A	1881	C	C3'-O3'	6.71	1.52	1.42
2	A	1874	C	C5'-C4'	6.70	1.61	1.51
4	D	71	ILE	C-N	6.69	1.38	1.33
6	G	9	ASP	CA-C	6.67	1.59	1.53
5	F	112	ASP	CA-CB	6.64	1.64	1.53
5	F	172	HIS	CA-C	6.63	1.61	1.52
2	A	2111	U	C3'-O3'	6.63	1.52	1.42
5	F	25	GLU	CA-CB	6.62	1.63	1.53
1	B	1289	A	C5'-C4'	6.59	1.61	1.51
2	A	2171	A	O3'-P	-6.57	1.51	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	111	PHE	N-CA	6.56	1.54	1.46
4	D	530	TYR	C-O	-6.54	1.16	1.24
6	G	159	ALA	C-N	6.49	1.42	1.33
4	D	57	LYS	N-CA	-6.48	1.38	1.46
6	G	4	HIS	CE1-NE2	6.48	1.39	1.32
6	G	45	ASP	N-CA	-6.47	1.37	1.46
5	F	96	GLY	N-CA	6.46	1.53	1.44
4	D	525	GLY	CA-C	-6.46	1.45	1.51
7	H	35	LEU	CA-C	6.46	1.60	1.52
2	A	2136	G	C2'-C1'	-6.45	1.43	1.53
8	I	87	PRO	CA-CB	6.44	1.61	1.54
4	D	14	VAL	CA-C	6.42	1.60	1.52
2	A	2161	C	P-O5'	-6.42	1.50	1.59
6	G	32	LYS	N-CA	-6.41	1.38	1.46
4	D	124	GLU	CA-C	-6.40	1.44	1.52
4	D	392	ASP	C-N	6.39	1.41	1.33
4	D	290	ARG	N-CA	6.39	1.54	1.46
7	H	47	ILE	CA-C	-6.38	1.45	1.52
3	E	25	U	C2'-C1'	6.38	1.62	1.53
8	I	121	ASN	CA-C	-6.36	1.45	1.53
5	F	183	ASP	N-CA	-6.35	1.38	1.46
4	D	506	ARG	CA-C	6.34	1.61	1.52
4	D	127	ARG	CD-NE	6.33	1.55	1.46
5	F	51	ASP	N-CA	-6.33	1.39	1.46
2	A	1852	U	C1'-N1	-6.33	1.39	1.48
2	A	1870	C	C5'-C4'	6.33	1.60	1.51
6	G	123	GLY	N-CA	6.31	1.54	1.45
2	A	1876	A	C5'-C4'	6.30	1.60	1.51
4	D	544	GLU	CA-C	6.30	1.60	1.53
4	D	131	ILE	CA-CB	-6.30	1.47	1.54
1	B	1294	G	C3'-C2'	-6.29	1.43	1.52
6	G	139	GLU	CA-C	-6.29	1.44	1.52
8	I	62	GLU	C-N	6.29	1.40	1.34
4	D	19	ARG	CA-CB	6.28	1.63	1.53
4	D	459	LEU	CA-C	6.27	1.61	1.52
5	F	14	LYS	CA-CB	6.25	1.63	1.53
6	G	132	ARG	CD-NE	6.25	1.54	1.46
3	E	42	C	C1'-N1	6.25	1.57	1.48
4	D	64	ARG	CD-NE	6.24	1.54	1.46
5	F	53	ARG	CD-NE	6.24	1.54	1.46
4	D	312	PHE	C-N	6.23	1.40	1.33
2	A	1866	A	C2'-C1'	-6.22	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1299	A	C1'-N9	6.22	1.56	1.47
4	D	519	LYS	CA-CB	6.20	1.61	1.53
5	F	165	ASN	N-CA	-6.20	1.37	1.45
8	I	104	VAL	C-N	6.19	1.42	1.33
2	A	2159	G	O3'-P	-6.18	1.51	1.61
2	A	1878	G	C4'-C3'	6.18	1.61	1.52
2	A	2186	G	C3'-O3'	6.17	1.51	1.42
2	A	1874	C	O3'-P	-6.16	1.51	1.61
4	D	219	ARG	CD-NE	6.16	1.54	1.46
2	A	2117	A	C5'-C4'	6.13	1.60	1.51
6	G	14	LYS	CA-CB	6.13	1.63	1.53
3	E	55	U	C5'-C4'	6.12	1.60	1.51
4	D	6	TYR	CA-CB	6.12	1.64	1.53
8	I	93	VAL	N-CA	6.12	1.53	1.46
6	G	123	GLY	C-N	-6.12	1.25	1.33
4	D	497	ILE	N-CA	-6.11	1.38	1.46
5	F	22	ASP	CA-CB	6.11	1.63	1.53
1	B	1303	C	P-O5'	-6.10	1.50	1.59
3	E	45	A	O3'-P	-6.09	1.52	1.61
4	D	53	ALA	N-CA	-6.06	1.38	1.46
2	A	1850	G	C1'-N9	6.05	1.57	1.48
4	D	50	ARG	CA-C	-6.04	1.44	1.52
2	A	2144	G	C5'-C4'	6.03	1.60	1.51
6	G	3	LEU	N-CA	6.03	1.53	1.46
2	A	1902	C	C3'-C2'	-6.02	1.43	1.52
6	G	98	PHE	CA-C	6.02	1.60	1.52
2	A	2160	C	C4'-O4'	6.01	1.54	1.45
2	A	2175	C	O4'-C1'	-6.00	1.32	1.41
3	E	69	C	C2'-C1'	-5.99	1.44	1.53
4	D	109	ALA	C-O	-5.99	1.17	1.24
6	G	82	TYR	CA-CB	5.98	1.63	1.52
4	D	166	GLY	CA-C	-5.97	1.45	1.52
2	A	2180	U	O3'-P	-5.97	1.52	1.61
4	D	240	TRP	CA-C	5.97	1.59	1.52
2	A	1888	G	P-O5'	-5.97	1.50	1.59
4	D	209	GLU	C-N	5.97	1.41	1.33
4	D	365	LEU	N-CA	5.96	1.53	1.46
4	D	506	ARG	CA-CB	5.95	1.62	1.53
4	D	510	HIS	C-N	5.95	1.41	1.33
4	D	315	PRO	CA-C	5.95	1.59	1.52
5	F	74	ARG	N-CA	-5.95	1.38	1.46
5	F	233	VAL	C-N	5.94	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2095	A	C3'-O3'	5.93	1.51	1.42
4	D	376	ASP	CA-C	-5.93	1.45	1.52
4	D	552	ARG	CD-NE	5.93	1.54	1.46
2	A	1885	A	C5'-C4'	5.93	1.60	1.51
4	D	9	HIS	ND1-CE1	5.90	1.38	1.32
3	E	39	A	C3'-C2'	-5.90	1.43	1.52
2	A	1835	G	P-O5'	-5.87	1.50	1.59
2	A	2107	G	P-O5'	-5.87	1.50	1.59
7	H	7	LYS	CA-C	-5.87	1.45	1.52
3	E	10	G	O4'-C1'	5.86	1.50	1.41
2	A	2151	U	O3'-P	-5.85	1.52	1.61
2	A	2187	U	C4'-C3'	5.84	1.61	1.52
4	D	20	HIS	ND1-CE1	5.84	1.38	1.32
4	D	189	PRO	N-CD	-5.83	1.39	1.47
2	A	2099	U	O3'-P	-5.83	1.52	1.61
5	F	222	VAL	CA-CB	-5.83	1.46	1.55
5	F	185	LEU	CA-C	5.82	1.60	1.52
8	I	110	ARG	CA-CB	5.82	1.60	1.53
3	E	52	C	O4'-C1'	-5.82	1.32	1.41
2	A	2145	C	C3'-C2'	5.80	1.61	1.52
8	I	51	GLN	CA-C	-5.79	1.45	1.52
2	A	1846	G	C5'-C4'	5.79	1.59	1.51
1	B	1239	A	C1'-N9	-5.79	1.38	1.47
5	F	219	GLY	C-N	5.78	1.40	1.33
4	D	194	ASP	C-O	-5.77	1.16	1.24
5	F	27	ILE	N-CA	-5.77	1.39	1.46
4	D	259	ALA	N-CA	-5.77	1.39	1.46
4	D	499	HIS	CA-CB	5.77	1.62	1.54
5	F	148	ASN	CA-C	5.76	1.59	1.52
5	F	188	ASN	C-N	5.76	1.41	1.33
2	A	2136	G	C5'-C4'	5.75	1.59	1.51
4	D	73	TYR	C-N	-5.75	1.27	1.33
8	I	126	ALA	CA-C	-5.75	1.45	1.52
2	A	2182	U	C1'-N1	5.72	1.57	1.48
4	D	465	MET	CA-C	-5.72	1.46	1.52
4	D	311	LEU	C-N	5.72	1.41	1.33
3	E	74	A	P-O5'	-5.71	1.51	1.59
5	F	32	GLU	N-CA	5.71	1.53	1.46
2	A	2182	U	O3'-P	-5.71	1.52	1.61
5	F	17	ALA	C-O	5.71	1.30	1.23
4	D	405	TRP	N-CA	-5.70	1.39	1.46
1	B	1334	G	O3'-P	-5.70	1.52	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	20	GLN	C-N	5.69	1.41	1.33
3	E	44	A	O5'-C5'	5.68	1.50	1.42
6	G	132	ARG	CZ-NH1	5.68	1.40	1.32
8	I	85	GLN	CA-C	5.68	1.60	1.52
4	D	345	SER	N-CA	-5.68	1.38	1.46
5	F	180	PHE	CA-C	-5.68	1.45	1.52
4	D	394	PHE	C-N	5.67	1.41	1.33
2	A	2127	G	O4'-C1'	5.67	1.50	1.41
2	A	2175	C	C5'-C4'	5.66	1.59	1.51
5	F	72	SER	C-O	-5.66	1.17	1.23
4	D	375	PRO	N-CA	-5.66	1.40	1.47
2	A	2155	U	C3'-O3'	5.65	1.50	1.42
2	A	1844	C	C2'-C1'	-5.65	1.44	1.53
6	G	19	PHE	C-N	5.64	1.41	1.33
4	D	283	ARG	CD-NE	5.63	1.54	1.46
2	A	1840	G	C1'-N9	-5.63	1.39	1.48
6	G	27	VAL	CA-C	-5.62	1.47	1.52
5	F	73	VAL	N-CA	5.61	1.53	1.46
2	A	1898	U	C5'-C4'	5.60	1.59	1.51
2	A	2159	G	C1'-N9	5.59	1.56	1.48
7	H	5	ARG	CD-NE	5.59	1.54	1.46
5	F	8	MET	CA-C	-5.58	1.45	1.52
2	A	2159	G	C5'-C4'	5.58	1.59	1.51
2	A	1888	G	O3'-P	-5.58	1.52	1.61
2	A	2124	G	P-O5'	-5.57	1.51	1.59
3	E	51	U	C1'-N1	5.57	1.56	1.48
3	E	70	C	C5'-C4'	5.56	1.59	1.51
4	D	511	ILE	CA-C	-5.56	1.45	1.52
2	A	1863	G	O3'-P	-5.56	1.52	1.61
7	H	20	TYR	CA-CB	5.55	1.62	1.53
2	A	2130	U	C2'-C1'	-5.54	1.45	1.53
1	B	1297	G	N9-C8	5.54	1.49	1.37
3	E	42	C	C5'-C4'	5.53	1.59	1.51
8	I	103	ILE	C-N	5.53	1.40	1.33
5	F	188	ASN	CA-CB	5.52	1.61	1.53
6	G	57	ALA	C-N	5.52	1.41	1.33
3	E	35	C	O5'-C5'	5.51	1.50	1.42
8	I	145	GLU	CA-CB	5.50	1.62	1.53
8	I	83	THR	CA-CB	5.50	1.63	1.53
3	E	45	A	C5'-C4'	5.49	1.59	1.51
2	A	2125	G	O5'-C5'	5.49	1.50	1.42
3	E	29	C	C1'-N1	5.49	1.56	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	225	ASP	CA-C	5.46	1.59	1.52
1	B	1295	U	C4'-C3'	-5.46	1.44	1.52
5	F	214	ILE	CA-C	5.46	1.59	1.52
2	A	1865	U	O3'-P	-5.46	1.52	1.61
5	F	138	PRO	C-N	5.46	1.39	1.33
1	B	1301	U	P-O5'	-5.45	1.51	1.59
4	D	477	ILE	N-CA	5.45	1.52	1.46
5	F	193	LEU	N-CA	-5.45	1.39	1.46
2	A	1900	A	O5'-C5'	5.44	1.51	1.42
2	A	2192	U	C5'-C4'	5.44	1.59	1.51
4	D	192	HIS	CG-CD2	5.44	1.41	1.35
7	H	10	LEU	C-N	5.44	1.40	1.33
6	G	15	LEU	CA-CB	5.42	1.61	1.53
4	D	401	SER	N-CA	-5.42	1.39	1.46
4	D	64	ARG	N-CA	5.42	1.53	1.46
3	E	36	A	N9-C4	-5.42	1.27	1.37
5	F	14	LYS	CA-C	5.41	1.60	1.52
1	B	1304	G	C4'-O4'	5.41	1.53	1.45
8	I	125	ASP	CA-C	5.41	1.60	1.52
4	D	228	TRP	N-CA	-5.41	1.39	1.45
4	D	309	ASN	CA-CB	5.40	1.62	1.53
2	A	2133	G	C5'-C4'	5.40	1.59	1.51
4	D	84	HIS	C-N	5.40	1.40	1.33
3	E	23	G	C4'-C3'	5.39	1.60	1.52
5	F	12	ARG	C-N	5.39	1.41	1.33
1	B	1237	C	O3'-P	-5.39	1.53	1.61
4	D	363	SER	N-CA	5.39	1.53	1.46
4	D	45	LYS	CA-C	5.37	1.59	1.52
4	D	532	GLU	C-O	-5.37	1.17	1.24
6	G	91	ARG	NE-CZ	5.36	1.39	1.33
1	B	1292	G	O3'-P	-5.36	1.53	1.61
4	D	70	LYS	CA-CB	5.35	1.61	1.53
4	D	274	GLU	N-CA	-5.35	1.39	1.46
6	G	127	TYR	C-N	-5.35	1.26	1.33
3	E	18	U	C4'-C3'	-5.34	1.44	1.52
4	D	466	LEU	CA-C	-5.34	1.46	1.52
4	D	306	ASN	CA-C	5.33	1.60	1.52
2	A	1868	C	O5'-C5'	5.33	1.50	1.42
4	D	10	ARG	CA-CB	5.33	1.61	1.53
2	A	1834	U	O3'-P	-5.32	1.53	1.61
1	B	1305	G	C4'-O4'	-5.29	1.37	1.45
1	B	1245	C	C4'-C3'	5.29	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	25	ILE	N-CA	-5.29	1.40	1.46
2	A	2174	C	C5'-C4'	5.29	1.59	1.51
3	E	5	G	O5'-C5'	5.29	1.50	1.42
4	D	175	ARG	C-N	5.28	1.40	1.33
2	A	2099	U	C2'-C1'	-5.28	1.45	1.53
2	A	2149	U	C4'-O4'	-5.28	1.37	1.45
6	G	106	ALA	CA-CB	5.28	1.61	1.53
6	G	106	ALA	N-CA	5.27	1.52	1.46
2	A	1873	G	P-O5'	-5.26	1.51	1.59
2	A	2124	G	C1'-N9	5.26	1.55	1.48
5	F	54	LYS	CA-CB	5.26	1.60	1.53
8	I	108	ARG	NE-CZ	5.25	1.38	1.33
8	I	127	ALA	CA-C	5.25	1.60	1.52
5	F	44	VAL	CA-C	-5.25	1.46	1.52
8	I	109	LYS	C-O	-5.25	1.17	1.24
3	E	68	C	N1-C2	-5.24	1.29	1.40
8	I	39	GLU	C-O	-5.24	1.17	1.24
3	E	28	U	C4'-C3'	5.23	1.60	1.52
6	G	4	HIS	N-CA	5.23	1.52	1.46
5	F	68	GLY	N-CA	-5.22	1.37	1.45
2	A	2165	C	P-O5'	-5.22	1.51	1.59
4	D	205	LEU	CB-CG	5.22	1.63	1.53
3	E	55	U	C2'-C1'	-5.22	1.45	1.53
7	H	27	ARG	C-N	5.21	1.41	1.33
7	H	44	GLN	N-CA	-5.21	1.39	1.45
5	F	30	LEU	CA-C	-5.21	1.46	1.52
2	A	2120	G	C3'-O3'	5.21	1.50	1.42
2	A	2171	A	O5'-C5'	5.20	1.50	1.42
2	A	2176	A	P-O5'	5.20	1.67	1.59
8	I	76	SER	CA-CB	5.19	1.59	1.52
6	G	150	GLY	CA-C	-5.19	1.46	1.51
8	I	46	LEU	C-N	5.19	1.40	1.33
6	G	73	VAL	C-O	-5.18	1.18	1.24
2	A	1879	C	C5'-C4'	5.18	1.59	1.51
3	E	30	G	C3'-C2'	5.18	1.60	1.52
5	F	140	PRO	C-N	-5.17	1.26	1.33
5	F	185	LEU	CA-CB	5.17	1.61	1.53
2	A	2191	A	O5'-C5'	5.17	1.50	1.42
4	D	491	PRO	C-N	5.17	1.39	1.33
4	D	428	VAL	CA-C	5.17	1.59	1.52
2	A	2153	C	C5'-C4'	5.16	1.59	1.51
2	A	1839	G	O3'-P	-5.16	1.53	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	60	GLU	CA-CB	5.16	1.61	1.53
4	D	423	PRO	C-N	-5.16	1.26	1.33
4	D	211	THR	N-CA	5.15	1.52	1.46
5	F	100	LEU	CA-C	5.15	1.59	1.52
3	E	43	G	O3'-P	-5.15	1.53	1.61
3	E	57	C	P-O5'	-5.15	1.52	1.59
2	A	2137	U	C4'-O4'	5.15	1.53	1.45
3	E	9	G	C4'-O4'	-5.15	1.38	1.45
8	I	9	ARG	N-CA	-5.15	1.39	1.46
5	F	56	ASP	CA-C	5.14	1.60	1.52
1	B	1242	G	C1'-N9	-5.14	1.40	1.48
3	E	59	A	C1'-N9	5.14	1.54	1.47
6	G	51	ASN	C-O	-5.14	1.17	1.24
4	D	214	ALA	CA-C	5.14	1.59	1.52
4	D	329	LEU	CA-C	-5.13	1.46	1.52
5	F	60	ARG	N-CA	-5.13	1.40	1.46
4	D	495	MET	C-N	5.13	1.40	1.33
3	E	6	G	C5'-C4'	5.12	1.58	1.51
4	D	262	GLU	N-CA	5.12	1.52	1.46
5	F	187	GLU	N-CA	-5.12	1.40	1.46
4	D	117	ASP	CA-C	5.12	1.59	1.52
4	D	377	SER	N-CA	5.12	1.52	1.46
5	F	77	VAL	CA-CB	-5.12	1.47	1.53
2	A	2143	C	C3'-C2'	5.11	1.60	1.52
2	A	2182	U	O4'-C1'	5.11	1.49	1.41
2	A	2149	U	C5'-C4'	5.11	1.58	1.51
4	D	31	PRO	N-CA	-5.10	1.41	1.47
8	I	1	PRO	C-N	5.09	1.40	1.33
4	D	117	ASP	N-CA	5.09	1.53	1.46
6	G	124	ARG	CA-C	-5.09	1.46	1.52
2	A	2106	U	C3'-O3'	5.08	1.49	1.42
4	D	415	MET	N-CA	-5.08	1.39	1.46
5	F	232	SER	CA-C	5.08	1.59	1.52
2	A	2151	U	C4'-C3'	5.08	1.60	1.52
2	A	2156	G	C2'-C1'	-5.08	1.45	1.53
2	A	2170	A	O5'-C5'	5.08	1.50	1.42
4	D	41	ASN	CA-CB	5.08	1.61	1.53
5	F	219	GLY	CA-C	-5.07	1.44	1.51
2	A	1858	A	C3'-O3'	5.07	1.49	1.42
2	A	2173	A	C2'-C1'	5.07	1.60	1.53
6	G	85	GLY	CA-C	-5.07	1.45	1.51
3	E	42	C	P-O5'	-5.06	1.52	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	146	ASP	CA-CB	5.06	1.61	1.53
5	F	58	ASN	CA-CB	5.05	1.59	1.53
6	G	28	PRO	N-CA	5.05	1.53	1.47
6	G	160	LYS	CA-CB	5.05	1.61	1.53
4	D	366	PHE	CA-CB	5.05	1.61	1.53
5	F	126	GLN	CA-C	5.04	1.59	1.52
6	G	157	THR	N-CA	-5.04	1.39	1.46
4	D	174	CYS	C-N	5.04	1.40	1.33
6	G	101	ARG	C-N	5.03	1.40	1.33
2	A	2172	U	O3'-P	-5.03	1.53	1.61
4	D	20	HIS	CB-CG	5.03	1.57	1.50
2	A	2178	C	O3'-P	-5.03	1.53	1.61
4	D	336	ARG	C-O	-5.03	1.18	1.24
5	F	19	LYS	C-N	5.03	1.40	1.33
2	A	2135	A	C1'-N9	-5.02	1.40	1.48
7	H	18	HIS	C-N	5.02	1.39	1.33
2	A	2188	U	O3'-P	-5.02	1.53	1.61
2	A	2124	G	O5'-C5'	5.02	1.50	1.42
4	D	71	ILE	CA-C	5.01	1.59	1.52
5	F	115	ILE	C-N	5.01	1.40	1.33
2	A	1851	U	C5'-C4'	5.01	1.58	1.51
5	F	74	ARG	CA-CB	5.01	1.59	1.53
4	D	23	LYS	CA-C	-5.00	1.46	1.52
4	D	48	LEU	C-N	5.00	1.40	1.33

All (841) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1871	A	P-O3'-C3'	13.59	140.58	120.20
8	I	91	ARG	NE-CZ-NH2	-13.12	107.39	119.20
2	A	2157	G	C2'-C3'-O3'	13.01	129.01	109.50
4	D	431	PHE	CA-CB-CG	-11.67	102.13	113.80
2	A	2158	A	P-O3'-C3'	11.27	137.11	120.20
4	D	99	ASN	CA-CB-CG	-10.77	101.83	112.60
7	H	39	ASP	O-C-N	-10.36	109.41	121.32
4	D	430	ARG	NE-CZ-NH1	10.36	131.85	121.50
6	G	137	PHE	CA-CB-CG	-10.12	103.67	113.80
2	A	2167	U	P-O5'-C5'	10.11	136.06	120.90
5	F	129	GLN	OE1-CD-NE2	-10.08	112.52	122.60
4	D	135	HIS	CA-CB-CG	-10.06	103.74	113.80
4	D	151	LEU	CA-C-N	9.99	136.54	122.36
4	D	151	LEU	C-N-CA	9.99	136.54	122.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	48	U	P-O3'-C3'	9.81	134.91	120.20
4	D	477	ILE	N-CA-C	9.72	120.53	110.62
5	F	119	ASP	CA-C-O	9.70	130.70	120.42
4	D	258	GLU	O-C-N	-9.46	112.09	122.12
4	D	314	PRO	N-CA-C	9.45	122.22	110.70
2	A	2111	U	O3'-P-O5'	-9.38	89.93	104.00
5	F	234	ASN	CA-CB-CG	9.38	121.97	112.60
2	A	2105	U	C4'-C3'-C2'	-9.33	93.27	102.60
4	D	186	LEU	N-CA-C	9.33	123.64	108.99
8	I	111	GLY	N-CA-C	9.16	122.41	112.33
4	D	285	SER	N-CA-C	9.12	122.20	111.71
4	D	224	ASN	CA-CB-CG	-9.11	103.49	112.60
4	D	498	SER	CA-C-O	9.11	131.03	121.38
6	G	5	ASP	CA-CB-CG	-9.08	103.52	112.60
6	G	121	PHE	CA-CB-CG	-9.07	104.73	113.80
2	A	2123	G	C4'-C3'-C2'	-9.01	93.59	102.60
4	D	432	ASN	CA-CB-CG	8.89	121.50	112.60
5	F	68	GLY	CA-C-N	8.88	136.75	120.95
5	F	68	GLY	C-N-CA	8.88	136.75	120.95
3	E	47	G	C4'-C3'-C2'	-8.87	93.73	102.60
7	H	42	VAL	CA-C-N	8.79	135.18	122.35
7	H	42	VAL	C-N-CA	8.79	135.18	122.35
5	F	119	ASP	O-C-N	-8.67	112.26	122.15
4	D	445	LEU	N-CA-C	8.66	122.45	110.24
4	D	119	ASP	CA-CB-CG	-8.62	103.98	112.60
2	A	2178	C	P-O3'-C3'	8.58	133.08	120.20
4	D	393	GLN	N-CA-C	8.54	121.36	111.11
7	H	25	ASN	CA-CB-CG	-8.47	104.13	112.60
4	D	490	PHE	CA-CB-CG	8.41	122.21	113.80
5	F	37	LYS	CB-CA-C	8.40	126.05	110.10
4	D	29	PHE	CA-CB-CG	-8.36	105.44	113.80
2	A	2145	C	C4'-C3'-C2'	-8.31	94.29	102.60
4	D	28	SER	O-C-N	-8.31	113.22	123.36
2	A	1835	G	P-O5'-C5'	8.29	133.34	120.90
3	E	35	C	C1'-O4'-C4'	8.28	118.18	109.90
4	D	548	ILE	N-CA-C	8.25	119.04	110.62
6	G	36	ASN	OD1-CG-ND2	-8.22	114.38	122.60
4	D	470	GLU	CA-C-N	8.18	128.13	119.05
4	D	470	GLU	C-N-CA	8.18	128.13	119.05
5	F	201	PRO	N-CA-CB	8.10	110.38	103.25
2	A	2164	C	O5'-C5'-C4'	-8.10	99.36	111.50
4	D	171	VAL	CB-CA-C	-8.06	101.65	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	434	LYS	CA-C-N	8.04	129.07	119.99
4	D	434	LYS	C-N-CA	8.04	129.07	119.99
8	I	69	ARG	O-C-N	-7.99	113.29	121.28
5	F	193	LEU	CA-C-O	-7.93	112.01	120.42
2	A	2119	A	C5'-C4'-C3'	7.89	127.03	115.20
4	D	20	HIS	CB-CG-CD2	-7.88	120.96	131.20
6	G	45	ASP	CA-C-N	7.85	131.13	120.54
6	G	45	ASP	C-N-CA	7.85	131.13	120.54
5	F	103	GLN	N-CA-C	7.83	122.41	113.01
5	F	89	ALA	CA-C-N	7.83	131.09	120.44
5	F	89	ALA	C-N-CA	7.83	131.09	120.44
4	D	139	ASN	OD1-CG-ND2	-7.81	114.79	122.60
4	D	81	ASN	CA-CB-CG	7.81	120.41	112.60
4	D	257	GLN	O-C-N	-7.80	113.66	122.09
7	H	39	ASP	CA-CB-CG	-7.78	104.82	112.60
2	A	1886	U	O4'-C1'-C2'	-7.77	99.83	107.60
4	D	30	PHE	CA-CB-CG	7.75	121.55	113.80
4	D	526	ASN	CA-CB-CG	-7.74	104.86	112.60
4	D	306	ASN	CA-CB-CG	-7.73	104.87	112.60
5	F	162	ARG	CA-CB-CG	7.71	129.51	114.10
6	G	150	GLY	CA-C-O	-7.70	113.77	121.93
4	D	276	VAL	CA-C-N	7.69	130.59	120.28
4	D	276	VAL	C-N-CA	7.69	130.59	120.28
2	A	2157	G	P-O3'-C3'	7.66	131.69	120.20
4	D	117	ASP	CA-C-N	7.66	130.87	120.38
4	D	117	ASP	C-N-CA	7.66	130.87	120.38
2	A	2166	U	C4'-C3'-C2'	-7.64	94.96	102.60
4	D	293	ARG	N-CA-CB	7.63	121.42	110.13
6	G	161	SER	O-C-N	-7.62	115.26	123.26
3	E	59	A	P-O5'-C5'	7.60	132.30	120.90
5	F	11	ILE	CA-C-N	7.59	131.21	120.28
5	F	11	ILE	C-N-CA	7.59	131.21	120.28
5	F	51	ASP	CA-C-N	7.58	130.44	120.28
5	F	51	ASP	C-N-CA	7.58	130.44	120.28
4	D	4	PHE	CB-CA-C	-7.57	99.16	110.67
6	G	122	ASP	O-C-N	-7.55	114.29	122.07
4	D	20	HIS	CB-CG-ND1	7.55	134.03	122.70
4	D	396	ASP	CA-CB-CG	-7.54	105.06	112.60
8	I	146	ALA	N-CA-C	7.53	119.12	111.07
4	D	434	LYS	O-C-N	-7.49	114.31	122.85
4	D	541	ASP	CA-C-N	7.46	130.28	120.28
4	D	541	ASP	C-N-CA	7.46	130.28	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	190	GLU	CA-C-N	7.44	130.25	120.28
5	F	190	GLU	C-N-CA	7.44	130.25	120.28
4	D	69	ILE	N-CA-C	7.43	119.68	109.80
5	F	181	ASP	CA-C-O	-7.41	113.69	121.55
5	F	148	ASN	N-CA-C	-7.41	97.36	108.99
8	I	63	VAL	O-C-N	-7.40	113.93	122.07
4	D	467	LEU	O-C-N	-7.40	113.96	122.84
7	H	29	LYS	CB-CA-C	-7.40	100.80	111.01
4	D	24	ASN	CA-CB-CG	-7.39	105.21	112.60
4	D	498	SER	O-C-N	-7.37	115.52	123.26
4	D	226	ALA	N-CA-C	7.36	119.52	110.91
8	I	57	GLU	CA-C-O	7.35	128.34	120.55
4	D	356	GLY	CA-C-N	7.31	127.27	120.03
4	D	356	GLY	C-N-CA	7.31	127.27	120.03
4	D	16	PRO	CA-C-N	7.30	126.83	119.24
4	D	16	PRO	C-N-CA	7.30	126.83	119.24
4	D	59	ILE	O-C-N	-7.30	114.77	123.02
4	D	139	ASN	N-CA-C	7.30	119.23	111.28
4	D	186	LEU	O-C-N	-7.28	115.10	123.33
5	F	104	ILE	N-CA-C	7.26	117.98	110.36
4	D	246	SER	CA-C-N	7.23	129.97	120.28
4	D	246	SER	C-N-CA	7.23	129.97	120.28
6	G	7	TYR	N-CA-C	7.23	118.85	110.97
2	A	2110	G	P-O3'-C3'	7.22	131.03	120.20
3	E	58	A	C1'-O4'-C4'	-7.21	102.69	109.90
4	D	270	GLU	N-CA-C	7.21	120.18	111.82
8	I	2	ARG	CA-C-N	7.21	132.75	120.71
8	I	2	ARG	C-N-CA	7.21	132.75	120.71
8	I	65	LEU	N-CA-C	7.19	119.12	111.28
6	G	9	ASP	CA-CB-CG	-7.18	105.42	112.60
8	I	34	LYS	CA-C-N	7.18	130.20	120.44
8	I	34	LYS	C-N-CA	7.18	130.20	120.44
7	H	45	HIS	CA-CB-CG	7.17	120.97	113.80
6	G	18	GLU	N-CA-C	-7.16	105.16	114.04
5	F	40	GLU	CA-C-N	7.15	132.58	122.72
5	F	40	GLU	C-N-CA	7.15	132.58	122.72
8	I	137	ARG	NE-CZ-NH1	7.15	128.65	121.50
4	D	326	VAL	O-C-N	-7.15	115.68	123.18
5	F	197	LYS	CA-C-N	7.14	130.72	120.79
5	F	197	LYS	C-N-CA	7.14	130.72	120.79
2	A	2152	G	P-O3'-C3'	7.14	130.91	120.20
8	I	145	GLU	N-CA-C	-7.13	104.56	113.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	216	THR	CA-C-N	7.13	130.79	120.38
5	F	216	THR	C-N-CA	7.13	130.79	120.38
6	G	155	ILE	N-CA-C	7.13	118.86	107.73
8	I	91	ARG	CA-C-N	7.13	128.75	119.84
8	I	91	ARG	C-N-CA	7.13	128.75	119.84
7	H	19	PHE	CA-CB-CG	7.12	120.92	113.80
5	F	24	ASN	OD1-CG-ND2	-7.12	115.48	122.60
4	D	394	PHE	CA-CB-CG	-7.11	106.69	113.80
3	E	76	C	P-O3'-C3'	7.10	130.86	120.20
4	D	326	VAL	CA-C-O	7.10	128.00	120.48
4	D	67	PRO	N-CA-C	7.09	122.73	113.86
6	G	56	LEU	CA-C-O	7.08	128.10	120.10
6	G	91	ARG	NE-CZ-NH1	-7.08	114.42	121.50
2	A	2174	C	C5'-C4'-C3'	-7.06	105.41	116.00
4	D	388	LEU	CA-C-O	7.04	129.59	121.28
2	A	2176	A	C4'-C3'-C2'	7.04	109.64	102.60
4	D	269	ILE	N-CA-C	7.04	117.80	110.62
6	G	88	VAL	CB-CA-C	-7.02	102.40	110.41
8	I	147	ASN	CA-CB-CG	-7.01	105.58	112.60
4	D	169	ARG	N-CA-C	7.01	118.92	111.28
3	E	7	G	P-O5'-C5'	7.00	131.40	120.90
5	F	124	VAL	N-CA-C	-7.00	104.37	110.74
6	G	47	LYS	CA-C-N	6.99	130.35	120.28
6	G	47	LYS	C-N-CA	6.99	130.35	120.28
2	A	2145	C	P-O3'-C3'	-6.99	109.72	120.20
6	G	4	HIS	CA-CB-CG	6.98	120.78	113.80
2	A	2116	G	P-O5'-C5'	6.97	131.35	120.90
6	G	136	ILE	CA-C-O	6.96	128.49	119.85
5	F	150	ALA	CA-C-N	6.96	130.18	120.29
5	F	150	ALA	C-N-CA	6.96	130.18	120.29
5	F	148	ASN	CA-CB-CG	-6.96	105.64	112.60
4	D	242	GLY	O-C-N	-6.95	115.73	124.00
7	H	36	LYS	O-C-N	-6.95	113.79	122.82
2	A	1872	A	P-O3'-C3'	6.95	130.62	120.20
5	F	36	ALA	CA-C-N	6.94	134.19	121.70
5	F	36	ALA	C-N-CA	6.94	134.19	121.70
4	D	482	ALA	N-CA-C	6.92	118.62	111.14
4	D	373	GLU	O-C-N	-6.92	116.00	123.26
3	E	34	U	C1'-O4'-C4'	-6.91	102.99	109.90
6	G	76	PHE	CA-C-O	-6.91	111.81	119.34
4	D	155	ASP	O-C-N	-6.91	113.41	122.59
4	D	420	THR	CB-CA-C	-6.91	98.06	109.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	115	MET	O-C-N	-6.89	114.35	122.20
8	I	110	ARG	NE-CZ-NH2	6.88	125.40	119.20
4	D	460	GLN	N-CA-C	6.88	120.77	112.38
6	G	70	ARG	O-C-N	-6.87	113.42	122.42
6	G	19	PHE	CA-C-N	6.86	131.88	122.07
6	G	19	PHE	C-N-CA	6.86	131.88	122.07
4	D	284	GLN	OE1-CD-NE2	-6.85	115.75	122.60
4	D	440	LYS	CB-CG-CD	6.85	127.05	111.30
2	A	1892	C	O4'-C1'-N1	6.84	118.77	108.50
5	F	99	ASP	CB-CA-C	-6.84	101.28	110.79
4	D	292	ALA	N-CA-C	6.83	120.09	111.69
4	D	301	GLU	N-CA-C	6.83	122.79	113.37
5	F	194	VAL	O-C-N	-6.83	114.80	121.83
3	E	17	C	O5'-C5'-C4'	6.82	121.73	111.50
6	G	36	ASN	O-C-N	-6.81	115.07	123.04
4	D	390	SER	N-CA-CB	6.78	121.71	110.52
5	F	7	ARG	CB-CA-C	-6.77	98.10	110.63
5	F	194	VAL	N-CA-CB	6.77	120.74	110.58
2	A	2153	C	C5'-C4'-C3'	-6.77	105.04	115.20
2	A	2187	U	O4'-C1'-N1	6.76	118.65	108.50
6	G	94	ARG	NE-CZ-NH2	-6.75	113.12	119.20
4	D	209	GLU	CA-C-N	6.74	133.84	121.70
4	D	209	GLU	C-N-CA	6.74	133.84	121.70
5	F	175	ILE	N-CA-C	6.73	118.34	111.00
4	D	146	ARG	N-CA-C	6.71	119.60	111.82
4	D	72	GLY	O-C-N	-6.70	118.45	123.61
4	D	527	PHE	CA-C-N	6.69	129.25	120.28
4	D	527	PHE	C-N-CA	6.69	129.25	120.28
2	A	2190	G	C5'-C4'-C3'	-6.69	105.97	116.00
3	E	43	G	C4'-C3'-C2'	-6.69	95.91	102.60
3	E	73	A	C3'-C2'-C1'	6.68	107.98	101.30
4	D	392	ASP	O-C-N	-6.68	114.43	122.65
4	D	379	THR	CA-C-N	6.67	131.97	123.10
4	D	379	THR	C-N-CA	6.67	131.97	123.10
2	A	2116	G	C4'-C3'-C2'	-6.67	95.94	102.60
4	D	405	TRP	CB-CG-CD1	6.65	136.87	126.90
4	D	219	ARG	NE-CZ-NH2	6.64	125.18	119.20
4	D	554	ALA	O-C-N	-6.63	115.17	122.92
6	G	176	PHE	CA-CB-CG	-6.63	107.17	113.80
2	A	1853	A	O3'-P-O5'	6.62	113.94	104.00
4	D	454	HIS	CE1-NE2-CD2	-6.62	102.38	109.00
5	F	136	LEU	N-CA-C	6.62	119.50	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	115	ASP	CA-CB-CG	-6.61	105.99	112.60
5	F	1	MET	CG-SD-CE	-6.61	86.37	100.90
2	A	2117	A	C5'-C4'-C3'	6.60	125.90	116.00
6	G	168	LEU	CA-C-N	6.60	129.45	120.54
6	G	168	LEU	C-N-CA	6.60	129.45	120.54
6	G	109	ARG	NE-CZ-NH1	-6.59	114.91	121.50
2	A	2101	A	C4'-C3'-C2'	-6.59	96.01	102.60
5	F	194	VAL	CA-C-N	6.59	129.00	120.44
5	F	194	VAL	C-N-CA	6.59	129.00	120.44
2	A	2136	G	C4'-C3'-C2'	-6.58	96.02	102.60
2	A	1906	G	P-O5'-C5'	-6.58	111.03	120.90
6	G	156	THR	CA-C-O	-6.57	113.50	120.80
5	F	213	SER	N-CA-C	-6.56	99.52	109.95
7	H	45	HIS	ND1-CE1-NE2	6.55	114.95	108.40
3	E	62	C	P-O3'-C3'	-6.55	110.37	120.20
2	A	2112	G	C5'-C4'-C3'	-6.55	106.18	116.00
7	H	45	HIS	CB-CG-CD2	-6.54	122.70	131.20
6	G	107	VAL	O-C-N	-6.53	113.65	121.10
7	H	43	ARG	NE-CZ-NH2	6.52	125.07	119.20
2	A	1837	C	P-O5'-C5'	-6.52	111.12	120.90
4	D	19	ARG	NE-CZ-NH2	-6.51	113.34	119.20
4	D	441	ARG	NH1-CZ-NH2	-6.51	110.84	119.30
4	D	405	TRP	CB-CG-CD2	-6.50	117.69	126.80
8	I	95	ARG	NE-CZ-NH1	6.50	128.00	121.50
4	D	424	SER	N-CA-C	6.49	118.44	111.36
6	G	88	VAL	CA-C-O	6.49	126.00	120.22
2	A	1884	G	P-O5'-C5'	6.49	130.63	120.90
8	I	43	TYR	CB-CG-CD1	6.48	130.53	120.80
6	G	135	ILE	N-CA-C	6.48	122.82	109.34
4	D	16	PRO	CA-C-O	-6.48	111.16	120.56
6	G	136	ILE	O-C-N	-6.48	113.56	122.05
4	D	83	GLU	O-C-N	-6.48	113.98	122.59
8	I	44	SER	N-CA-C	6.47	119.16	111.33
4	D	282	GLY	CA-C-N	6.46	133.88	121.54
4	D	282	GLY	C-N-CA	6.46	133.88	121.54
5	F	75	VAL	CG1-CB-CG2	-6.46	96.59	110.80
5	F	103	GLN	CB-CG-CD	6.46	123.58	112.60
6	G	132	ARG	N-CA-C	6.45	118.39	111.36
4	D	124	GLU	CA-C-N	6.43	128.90	120.28
4	D	124	GLU	C-N-CA	6.43	128.90	120.28
4	D	104	LEU	CA-C-N	6.42	129.41	120.29
4	D	104	LEU	C-N-CA	6.42	129.41	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2164	C	P-O3'-C3'	6.42	129.84	120.20
5	F	151	GLU	CB-CA-C	-6.42	99.93	110.85
5	F	184	LYS	CA-C-O	6.40	127.20	120.42
4	D	348	LYS	CG-CD-CE	6.40	126.02	111.30
2	A	2130	U	P-O3'-C3'	-6.39	110.62	120.20
5	F	212	VAL	CA-C-O	6.39	127.55	120.59
2	A	1861	G	C4'-C3'-C2'	-6.38	96.22	102.60
2	A	1859	U	C5'-C4'-C3'	-6.38	106.43	116.00
2	A	2109	U	C4'-C3'-C2'	-6.38	96.22	102.60
6	G	78	ILE	N-CA-C	6.37	122.60	109.34
2	A	1862	G	C5'-C4'-C3'	-6.37	106.44	116.00
5	F	177	LYS	N-CA-CB	-6.37	100.59	110.46
4	D	2	ALA	N-CA-CB	-6.36	100.86	110.40
8	I	26	VAL	CA-CB-CG2	6.36	121.22	110.40
2	A	2177	C	O5'-C5'-C4'	-6.36	101.96	111.50
4	D	404	VAL	CB-CA-C	-6.36	103.83	111.97
7	H	42	VAL	CA-C-O	6.35	127.11	120.25
4	D	152	ARG	NE-CZ-NH2	-6.34	113.49	119.20
5	F	144	THR	CA-CB-CG2	6.34	121.27	110.50
5	F	139	ASN	CA-C-N	6.33	126.02	119.56
5	F	139	ASN	C-N-CA	6.33	126.02	119.56
2	A	2176	A	C1'-O4'-C4'	6.32	116.22	109.90
6	G	152	ASP	CA-CB-CG	6.32	118.92	112.60
8	I	5	VAL	O-C-N	-6.32	115.93	122.63
4	D	304	LYS	CA-C-N	6.32	131.27	120.72
4	D	304	LYS	C-N-CA	6.32	131.27	120.72
2	A	2169	A	O4'-C1'-N9	6.31	117.96	108.50
8	I	105	GLU	CA-C-N	6.31	128.64	120.44
8	I	105	GLU	C-N-CA	6.31	128.64	120.44
4	D	273	LEU	CA-C-N	6.31	128.73	120.28
4	D	273	LEU	C-N-CA	6.31	128.73	120.28
5	F	145	VAL	CA-C-N	6.30	129.15	120.39
5	F	145	VAL	C-N-CA	6.30	129.15	120.39
6	G	19	PHE	CA-C-O	6.30	126.72	119.35
4	D	531	GLU	N-CA-C	6.29	118.14	111.28
5	F	188	ASN	CA-C-N	6.29	128.95	120.65
5	F	188	ASN	C-N-CA	6.29	128.95	120.65
8	I	11	ILE	N-CA-C	6.29	118.69	109.63
2	A	1857	G	C4'-C3'-C2'	-6.28	96.32	102.60
4	D	28	SER	CA-C-O	6.28	128.01	120.28
8	I	110	ARG	NH1-CZ-NH2	-6.27	111.14	119.30
4	D	339	ILE	N-CA-C	-6.27	99.17	108.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	283	ARG	NE-CZ-NH1	6.27	127.77	121.50
4	D	479	THR	CA-C-N	6.26	128.58	120.44
4	D	479	THR	C-N-CA	6.26	128.58	120.44
2	A	2109	U	C5'-C4'-O4'	6.26	119.19	109.80
4	D	208	PHE	N-CA-C	6.25	124.12	110.80
2	A	2109	U	O4'-C1'-N1	6.24	117.86	108.50
5	F	52	ALA	N-CA-C	6.24	118.08	111.28
3	E	20	G	C5'-C4'-C3'	-6.23	105.86	115.20
3	E	3	C	C5'-C4'-C3'	-6.22	106.67	116.00
4	D	363	SER	N-CA-CB	6.21	119.78	110.22
1	B	1294	G	P-O5'-C5'	6.20	130.20	120.90
4	D	191	ASN	CA-CB-CG	-6.20	106.40	112.60
5	F	112	ASP	N-CA-CB	6.20	119.31	110.13
4	D	66	GLN	CA-C-O	-6.20	113.56	120.25
4	D	163	LEU	N-CA-C	6.19	119.60	109.76
8	I	4	ARG	NE-CZ-NH2	-6.19	113.63	119.20
8	I	141	HIS	ND1-CE1-NE2	6.18	114.58	108.40
2	A	2162	G	P-O3'-C3'	-6.18	110.93	120.20
2	A	2094	A	P-O5'-C5'	6.18	130.17	120.90
4	D	540	ALA	CA-C-N	6.17	129.17	120.28
4	D	540	ALA	C-N-CA	6.17	129.17	120.28
5	F	139	ASN	O-C-N	-6.17	117.76	121.71
8	I	67	ASN	CA-CB-CG	-6.15	106.45	112.60
8	I	85	GLN	N-CA-CB	6.15	119.48	109.95
3	E	38	A	P-O5'-C5'	-6.15	111.68	120.90
6	G	91	ARG	NE-CZ-NH2	6.14	124.72	119.20
1	B	1240	U	C5'-C4'-C3'	-6.13	106.00	115.20
2	A	1888	G	P-O5'-C5'	6.13	130.09	120.90
4	D	285	SER	CA-C-O	6.12	127.02	120.10
8	I	61	PHE	N-CA-C	-6.12	106.42	114.31
8	I	141	HIS	CE1-NE2-CD2	-6.10	102.90	109.00
1	B	1290	G	O4'-C1'-N9	6.10	117.65	108.50
5	F	67	HIS	CE1-NE2-CD2	-6.10	102.90	109.00
2	A	1859	U	O3'-P-O5'	-6.10	94.85	104.00
8	I	141	HIS	N-CA-C	6.10	117.80	111.03
4	D	280	THR	N-CA-CB	6.09	118.78	110.38
6	G	56	LEU	O-C-N	-6.09	115.10	122.22
4	D	388	LEU	O-C-N	-6.09	116.10	123.10
5	F	81	GLY	N-CA-C	6.09	122.88	111.80
4	D	24	ASN	N-CA-C	6.08	119.81	111.54
6	G	67	THR	O-C-N	-6.08	115.92	122.85
4	D	32	GLY	CA-C-N	6.08	129.39	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	32	GLY	C-N-CA	6.08	129.39	120.82
4	D	186	LEU	CA-C-O	6.08	127.80	120.99
5	F	214	ILE	CB-CA-C	6.07	121.22	110.71
8	I	110	ARG	CA-C-N	6.07	127.06	120.44
8	I	110	ARG	C-N-CA	6.07	127.06	120.44
2	A	2145	C	C1'-O4'-C4'	-6.07	103.83	109.90
5	F	103	GLN	CA-C-N	6.07	128.43	120.60
5	F	103	GLN	C-N-CA	6.07	128.43	120.60
2	A	1881	C	P-O5'-C5'	6.06	129.99	120.90
6	G	85	GLY	CA-C-O	-6.06	115.87	121.63
3	E	69	C	C4'-C3'-C2'	-6.06	96.54	102.60
4	D	408	VAL	O-C-N	-6.05	113.86	121.84
4	D	461	VAL	CB-CA-C	-6.04	101.38	111.29
6	G	109	ARG	NE-CZ-NH2	6.04	124.63	119.20
2	A	1834	U	P-O5'-C5'	6.03	129.95	120.90
8	I	108	ARG	CG-CD-NE	-6.03	98.73	112.00
5	F	92	ALA	O-C-N	-6.03	115.89	123.01
2	A	1871	A	P-O5'-C5'	-6.03	111.86	120.90
5	F	24	ASN	CA-CB-CG	-6.02	106.58	112.60
6	G	28	PRO	CA-C-O	-6.02	114.76	121.32
4	D	251	LYS	CA-C-O	6.02	126.93	120.55
4	D	529	GLU	N-CA-C	6.01	117.92	111.36
2	A	2114	A	P-O3'-C3'	-6.00	111.19	120.20
4	D	298	ASN	CA-C-O	-6.00	115.47	122.37
1	B	1240	U	C4'-C3'-O3'	6.00	118.40	109.40
2	A	2110	G	C3'-C2'-C1'	-5.99	95.51	101.50
4	D	486	ALA	CA-C-O	5.99	126.90	120.55
5	F	87	ALA	CA-C-N	5.99	128.30	120.28
5	F	87	ALA	C-N-CA	5.99	128.30	120.28
4	D	518	GLY	CA-C-O	5.98	125.66	119.02
8	I	108	ARG	CD-NE-CZ	-5.98	116.02	124.40
5	F	41	SER	N-CA-CB	5.97	120.17	110.43
5	F	219	GLY	N-CA-C	-5.97	99.03	113.18
8	I	17	PHE	N-CA-C	-5.97	106.03	113.55
4	D	155	ASP	CA-CB-CG	-5.97	106.63	112.60
2	A	1874	C	O4'-C1'-N1	5.96	117.44	108.50
4	D	445	LEU	O-C-N	-5.96	115.69	122.97
4	D	507	ILE	CA-C-N	-5.96	114.25	122.30
4	D	507	ILE	C-N-CA	-5.96	114.25	122.30
4	D	19	ARG	N-CA-C	-5.96	100.33	108.38
5	F	130	VAL	O-C-N	-5.96	116.73	123.10
4	D	246	SER	O-C-N	-5.96	114.45	122.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	441	ARG	NE-CZ-NH2	5.95	124.56	119.20
5	F	187	GLU	N-CA-C	5.95	118.25	111.11
2	A	2165	C	C4'-C3'-O3'	-5.95	104.07	113.00
4	D	214	ALA	CA-C-N	5.95	129.93	121.96
4	D	214	ALA	C-N-CA	5.95	129.93	121.96
3	E	66	C	C1'-C2'-O2'	5.94	117.31	108.40
2	A	2140	G	C4'-C3'-C2'	-5.94	96.66	102.60
8	I	49	LEU	N-CA-C	-5.94	103.58	111.24
5	F	26	ALA	N-CA-C	5.93	117.42	111.07
4	D	496	VAL	CG1-CB-CG2	-5.93	97.76	110.80
8	I	134	VAL	CA-C-O	5.92	127.21	121.05
4	D	258	GLU	N-CA-C	5.92	117.74	111.28
4	D	168	ARG	NE-CZ-NH1	5.92	127.42	121.50
4	D	333	TYR	N-CA-CB	5.91	120.45	110.69
4	D	470	GLU	O-C-N	-5.91	114.52	121.32
6	G	148	VAL	N-CA-C	5.91	117.25	109.21
2	A	2148	G	C4'-C3'-C2'	-5.91	96.69	102.60
4	D	280	THR	N-CA-C	-5.90	102.20	110.35
5	F	97	MET	CG-SD-CE	-5.90	87.91	100.90
4	D	176	LEU	O-C-N	5.90	128.23	122.09
4	D	302	TYR	N-CA-C	5.90	117.38	111.07
4	D	352	VAL	CB-CA-C	-5.90	102.90	110.98
8	I	44	SER	CA-C-N	5.90	128.46	120.44
8	I	44	SER	C-N-CA	5.90	128.46	120.44
6	G	58	ALA	CA-C-O	-5.88	114.19	120.42
4	D	474	ASP	CA-C-N	5.87	129.62	120.75
4	D	474	ASP	C-N-CA	5.87	129.62	120.75
2	A	2145	C	C2'-C3'-O3'	5.87	122.51	113.70
4	D	200	TRP	CD2-CE2-CZ2	-5.87	116.53	122.40
3	E	43	G	C1'-O4'-C4'	-5.87	104.03	109.90
4	D	140	LEU	N-CA-C	5.86	123.28	110.80
2	A	2177	C	O4'-C1'-N1	5.86	117.28	108.50
4	D	221	PHE	CA-C-N	5.85	129.96	120.60
4	D	221	PHE	C-N-CA	5.85	129.96	120.60
6	G	73	VAL	O-C-N	-5.85	116.94	123.26
6	G	124	ARG	CA-C-O	5.85	126.72	120.70
5	F	134	ARG	NE-CZ-NH2	5.84	124.46	119.20
6	G	89	THR	O-C-N	-5.84	115.76	122.89
2	A	2159	G	C5'-C4'-C3'	-5.84	107.24	116.00
1	B	1304	G	P-O3'-C3'	5.84	128.96	120.20
4	D	481	ARG	NH1-CZ-NH2	-5.84	111.71	119.30
4	D	395	ARG	CG-CD-NE	-5.83	99.16	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2141	G	C3'-C2'-C1'	-5.82	95.48	101.30
2	A	2126	A	P-O3'-C3'	5.82	128.93	120.20
5	F	212	VAL	O-C-N	-5.82	115.29	122.97
5	F	48	LEU	N-CA-C	5.81	118.25	109.41
4	D	368	MET	N-CA-CB	5.81	118.75	110.16
4	D	206	HIS	CA-CB-CG	-5.81	107.99	113.80
4	D	173	LEU	N-CA-C	5.80	117.28	111.07
3	E	23	G	P-O5'-C5'	5.80	129.60	120.90
4	D	362	LYS	CA-C-N	5.80	128.63	120.28
4	D	362	LYS	C-N-CA	5.80	128.63	120.28
4	D	366	PHE	O-C-N	-5.80	115.98	122.12
5	F	119	ASP	CA-CB-CG	-5.79	106.81	112.60
6	G	153	ILE	CA-CB-CG1	5.79	120.25	110.40
4	D	31	PRO	CA-C-O	-5.79	114.36	121.31
4	D	395	ARG	NE-CZ-NH2	-5.79	113.99	119.20
1	B	1300	G	P-O5'-C5'	5.78	129.57	120.90
4	D	221	PHE	CA-C-O	5.78	126.89	120.82
6	G	47	LYS	O-C-N	-5.77	114.60	122.33
3	E	48	U	C2'-C3'-O3'	5.76	122.34	113.70
3	E	52	C	P-O5'-C5'	-5.76	112.26	120.90
4	D	69	ILE	CB-CA-C	-5.75	103.34	111.28
5	F	163	TYR	O-C-N	-5.75	116.37	123.33
4	D	499	HIS	ND1-CE1-NE2	5.75	114.15	108.40
8	I	109	LYS	CA-C-N	5.75	130.62	121.66
8	I	109	LYS	C-N-CA	5.75	130.62	121.66
5	F	160	GLN	OE1-CD-NE2	5.75	128.34	122.60
4	D	82	PRO	CA-C-N	5.74	132.51	121.54
4	D	82	PRO	C-N-CA	5.74	132.51	121.54
2	A	2131	U	P-O3'-C3'	5.74	128.81	120.20
4	D	490	PHE	N-CA-C	5.74	118.00	110.08
3	E	49	C	P-O3'-C3'	5.73	128.80	120.20
4	D	164	SER	CA-C-N	5.73	132.64	121.41
4	D	164	SER	C-N-CA	5.73	132.64	121.41
4	D	87	ARG	NE-CZ-NH1	5.73	127.23	121.50
5	F	221	GLY	CA-C-N	5.73	131.02	123.17
5	F	221	GLY	C-N-CA	5.73	131.02	123.17
2	A	2133	G	P-O3'-C3'	5.73	128.79	120.20
4	D	104	LEU	O-C-N	-5.73	115.52	122.22
4	D	153	LEU	CA-C-O	-5.72	115.45	120.60
4	D	307	GLU	O-C-N	-5.72	116.06	122.12
5	F	172	HIS	O-C-N	-5.71	116.71	123.22
1	B	1335	U	O5'-C5'-C4'	5.71	120.26	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1902	C	C4'-C3'-C2'	-5.71	96.89	102.60
4	D	139	ASN	CA-CB-CG	5.70	118.30	112.60
6	G	79	ARG	O-C-N	-5.70	116.75	123.25
1	B	1292	G	P-O3'-C3'	5.70	128.75	120.20
8	I	88	VAL	CA-C-O	-5.70	115.99	121.63
4	D	533	TYR	CA-C-N	5.70	127.91	120.28
4	D	533	TYR	C-N-CA	5.70	127.91	120.28
2	A	2119	A	N9-C1'-C2'	-5.70	105.46	114.00
4	D	117	ASP	CA-CB-CG	5.70	118.30	112.60
5	F	75	VAL	N-CA-C	5.70	116.08	108.11
1	B	1244	G	C1'-C2'-O2'	5.68	116.92	108.40
3	E	5	G	P-O5'-C5'	-5.68	112.38	120.90
1	B	1292	G	C3'-C2'-O2'	5.68	119.22	110.70
4	D	477	ILE	O-C-N	-5.67	116.36	121.87
5	F	3	LYS	CA-C-N	5.67	132.38	121.54
5	F	3	LYS	C-N-CA	5.67	132.38	121.54
4	D	146	ARG	CA-C-N	5.67	128.34	120.29
4	D	146	ARG	C-N-CA	5.67	128.34	120.29
6	G	88	VAL	O-C-N	-5.66	117.88	122.97
1	B	1242	G	C4'-C3'-C2'	-5.66	96.94	102.60
1	B	1298	U	C5'-C4'-C3'	5.65	123.68	115.20
4	D	512	LEU	CB-CA-C	-5.65	101.58	110.79
8	I	95	ARG	CD-NE-CZ	5.65	132.31	124.40
4	D	107	VAL	O-C-N	-5.64	116.40	121.87
4	D	316	GLY	CA-C-O	-5.64	113.45	121.52
4	D	388	LEU	CA-C-N	5.64	130.93	122.47
4	D	388	LEU	C-N-CA	5.64	130.93	122.47
5	F	210	LYS	CA-C-N	5.64	130.72	122.77
5	F	210	LYS	C-N-CA	5.64	130.72	122.77
4	D	262	GLU	CA-CB-CG	5.64	125.38	114.10
4	D	348	LYS	N-CA-CB	5.63	118.25	109.97
2	A	2142	A	P-O5'-C5'	-5.63	112.45	120.90
5	F	112	ASP	N-CA-C	-5.63	104.53	111.40
1	B	1303	C	C4'-C3'-O3'	-5.63	104.56	113.00
4	D	125	GLN	CA-C-O	-5.62	114.59	120.55
4	D	218	ASP	CA-C-O	5.62	126.51	120.38
5	F	145	VAL	CB-CA-C	-5.62	105.15	111.45
8	I	105	GLU	O-C-N	-5.62	116.16	122.12
4	D	484	GLU	CA-C-N	5.62	127.81	120.28
4	D	484	GLU	C-N-CA	5.62	127.81	120.28
5	F	102	ASP	CA-C-O	5.62	126.48	119.12
2	A	2126	A	C4'-C3'-O3'	5.61	117.82	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	5	VAL	N-CA-C	5.61	117.71	109.63
4	D	327	SER	CA-C-N	5.61	130.09	122.07
4	D	327	SER	C-N-CA	5.61	130.09	122.07
3	E	69	C	C1'-C2'-O2'	5.61	116.81	108.40
6	G	43	ILE	CB-CA-C	5.60	119.55	111.65
2	A	2115	G	O4'-C1'-N9	5.59	116.89	108.50
4	D	459	LEU	N-CA-C	5.59	119.94	113.18
2	A	1894	C	C4'-C3'-O3'	-5.59	104.62	113.00
6	G	132	ARG	CA-C-O	5.58	126.33	120.42
4	D	236	GLU	CA-C-O	5.58	127.33	120.92
5	F	67	HIS	CA-CB-CG	-5.58	108.22	113.80
8	I	29	LEU	N-CA-C	5.58	118.12	111.71
2	A	1843	C	O4'-C1'-N1	5.57	116.86	108.50
4	D	200	TRP	CH2-CZ2-CE2	5.57	124.75	117.50
1	B	1303	C	P-O5'-C5'	5.57	129.26	120.90
4	D	481	ARG	NE-CZ-NH1	5.57	127.06	121.50
4	D	499	HIS	CE1-NE2-CD2	-5.56	103.44	109.00
4	D	340	ASP	CA-CB-CG	5.56	118.16	112.60
3	E	50	G	O5'-C5'-C4'	5.56	119.84	111.50
4	D	113	ASP	CA-C-O	-5.55	115.11	119.66
5	F	207	VAL	CA-C-N	5.54	131.07	122.26
5	F	207	VAL	C-N-CA	5.54	131.07	122.26
2	A	2148	G	P-O3'-C3'	5.54	128.51	120.20
4	D	53	ALA	O-C-N	-5.54	114.34	122.43
4	D	84	HIS	CA-C-N	5.54	127.64	120.44
4	D	84	HIS	C-N-CA	5.54	127.64	120.44
2	A	2103	C	C4'-C3'-O3'	-5.53	104.70	113.00
2	A	1860	G	O4'-C1'-N9	5.53	116.79	108.50
5	F	17	ALA	N-CA-CB	-5.53	101.52	110.81
2	A	2175	C	O5'-C5'-C4'	5.53	119.79	111.50
4	D	249	GLU	CA-C-N	5.53	128.14	120.29
4	D	249	GLU	C-N-CA	5.53	128.14	120.29
7	H	6	GLU	N-CA-CB	5.53	118.16	110.04
3	E	2	G	P-O3'-C3'	-5.52	111.92	120.20
3	E	5	G	C4'-C3'-C2'	-5.52	97.08	102.60
5	F	128	GLY	CA-C-N	5.52	129.96	121.19
5	F	128	GLY	C-N-CA	5.52	129.96	121.19
5	F	171	ILE	N-CA-CB	5.52	118.62	111.83
4	D	9	HIS	CE1-NE2-CD2	-5.51	103.49	109.00
3	E	19	G	C3'-C2'-C1'	5.51	107.01	101.50
3	E	22	A	C5'-C4'-C3'	-5.51	107.73	116.00
5	F	90	ALA	N-CA-C	5.51	117.09	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	52	ARG	NE-CZ-NH1	5.50	127.00	121.50
1	B	1237	C	O3'-P-O5'	-5.50	95.75	104.00
6	G	116	LEU	O-C-N	-5.50	116.68	123.44
5	F	188	ASN	OD1-CG-ND2	-5.50	117.10	122.60
6	G	122	ASP	CA-C-N	5.49	132.17	121.41
6	G	122	ASP	C-N-CA	5.49	132.17	121.41
4	D	221	PHE	CA-CB-CG	-5.49	108.31	113.80
1	B	1335	U	C5'-C4'-O4'	5.49	117.33	109.10
2	A	2153	C	O4'-C1'-N1	5.49	116.43	108.20
4	D	128	LEU	O-C-N	-5.49	115.89	122.15
3	E	72	C	C5'-C4'-O4'	-5.49	101.57	109.80
8	I	23	ALA	N-CA-C	5.49	117.69	111.11
2	A	1842	G	C1'-C2'-O2'	5.48	116.63	108.40
4	D	420	THR	N-CA-C	5.48	118.34	108.48
8	I	35	LYS	N-CA-C	-5.47	105.23	111.14
8	I	39	GLU	CA-C-N	5.47	129.89	121.19
8	I	39	GLU	C-N-CA	5.47	129.89	121.19
4	D	391	VAL	N-CA-C	5.47	116.42	107.24
3	E	19	G	O4'-C4'-C3'	5.46	111.56	106.10
6	G	122	ASP	CA-C-O	5.46	126.56	120.82
2	A	2141	G	P-O3'-C3'	-5.46	112.01	120.20
4	D	84	HIS	CB-CG-CD2	-5.46	124.11	131.20
4	D	212	VAL	CB-CA-C	-5.46	102.36	110.33
3	E	38	A	O4'-C1'-C2'	-5.46	102.14	107.60
5	F	157	LYS	N-CA-C	5.45	117.93	111.33
6	G	126	ASN	OD1-CG-ND2	5.45	128.05	122.60
4	D	254	ARG	CA-C-O	-5.45	115.08	120.70
3	E	72	C	C1'-O4'-C4'	-5.45	104.45	109.90
6	G	145	VAL	N-CA-C	5.45	117.05	109.80
2	A	1880	U	C2'-C3'-O3'	5.45	121.87	113.70
5	F	74	ARG	N-CA-C	5.45	117.51	108.20
8	I	80	GLY	N-CA-C	-5.45	100.27	113.18
4	D	479	THR	O-C-N	-5.44	115.95	122.15
3	E	76	C	C3'-C2'-O2'	5.44	118.86	110.70
4	D	172	ALA	CB-CA-C	-5.44	101.76	110.79
4	D	454	HIS	N-CA-C	5.44	116.89	111.07
8	I	19	SER	N-CA-C	5.44	118.20	110.10
4	D	358	ASN	OD1-CG-ND2	5.44	128.04	122.60
4	D	175	ARG	CA-C-N	5.43	127.87	120.54
4	D	175	ARG	C-N-CA	5.43	127.87	120.54
4	D	35	ILE	CA-C-O	5.42	126.08	120.39
2	A	2165	C	O4'-C1'-N1	5.42	116.63	108.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	74	LEU	CA-C-N	5.42	125.89	120.52
4	D	74	LEU	C-N-CA	5.42	125.89	120.52
8	I	118	ARG	CB-CG-CD	5.42	123.76	111.30
2	A	2109	U	C5'-C4'-C3'	-5.40	107.89	116.00
4	D	242	GLY	N-CA-C	5.40	117.33	110.20
4	D	314	PRO	O-C-N	-5.40	115.08	121.46
5	F	54	LYS	N-CA-C	5.40	119.43	112.41
5	F	231	ALA	N-CA-C	5.40	118.73	110.20
3	E	30	G	O4'-C1'-C2'	-5.40	102.20	107.60
6	G	36	ASN	CB-CG-OD1	5.40	131.60	120.80
5	F	50	ILE	CA-C-N	5.40	130.96	122.49
5	F	50	ILE	C-N-CA	5.40	130.96	122.49
6	G	124	ARG	N-CA-C	5.39	116.97	111.14
4	D	191	ASN	CA-C-N	5.39	130.51	122.74
4	D	191	ASN	C-N-CA	5.39	130.51	122.74
6	G	177	ARG	O-C-N	-5.39	117.60	123.26
6	G	12	VAL	O-C-N	-5.39	116.28	121.83
4	D	398	MET	N-CA-C	5.39	117.58	111.11
6	G	39	VAL	O-C-N	-5.38	115.84	122.57
8	I	49	LEU	CB-CA-C	5.38	119.74	110.86
4	D	108	TYR	CB-CG-CD2	-5.38	112.73	120.80
6	G	148	VAL	CA-CB-CG1	5.37	119.53	110.40
8	I	126	ALA	CA-C-N	5.37	129.19	120.60
8	I	126	ALA	C-N-CA	5.37	129.19	120.60
2	A	1897	G	P-O5'-C5'	-5.36	112.86	120.90
2	A	2131	U	C3'-C2'-C1'	-5.36	96.14	101.50
8	I	135	LYS	CA-C-O	-5.36	115.18	121.07
4	D	21	ILE	O-C-N	-5.35	115.86	122.18
4	D	423	PRO	CA-C-O	-5.35	115.50	121.23
2	A	2164	C	C3'-C2'-C1'	5.35	106.65	101.30
4	D	430	ARG	NH1-CZ-NH2	-5.35	112.35	119.30
6	G	88	VAL	N-CA-CB	5.34	119.29	112.34
6	G	121	PHE	CA-C-O	5.34	126.47	120.70
8	I	14	ASP	O-C-N	-5.34	116.66	121.31
2	A	2183	A	O4'-C1'-N9	5.34	116.51	108.50
4	D	477	ILE	CB-CA-C	-5.34	104.93	112.14
1	B	1245	C	C4'-C3'-C2'	-5.34	97.26	102.60
2	A	2121	G	P-O3'-C3'	-5.34	112.20	120.20
6	G	47	LYS	N-CA-C	5.34	118.95	112.23
5	F	158	ALA	N-CA-C	5.33	116.90	111.14
4	D	53	ALA	CA-C-O	5.33	125.94	119.11
1	B	1294	G	C3'-C2'-O2'	5.33	118.69	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1853	A	P-O5'-C5'	-5.33	112.91	120.90
4	D	510	HIS	CG-CD2-NE2	5.33	112.53	107.20
5	F	35	THR	N-CA-CB	5.33	118.91	110.87
2	A	1850	G	P-O5'-C5'	5.32	128.88	120.90
7	H	42	VAL	O-C-N	-5.32	114.53	121.82
4	D	364	THR	O-C-N	-5.32	115.73	122.27
6	G	155	ILE	O-C-N	-5.32	116.18	122.77
5	F	110	ASN	OD1-CG-ND2	-5.31	117.29	122.60
4	D	303	GLN	OE1-CD-NE2	-5.31	117.29	122.60
8	I	65	LEU	CA-C-N	5.31	127.39	120.28
8	I	65	LEU	C-N-CA	5.31	127.39	120.28
8	I	58	LEU	CA-C-N	5.29	131.66	121.18
8	I	58	LEU	C-N-CA	5.29	131.66	121.18
4	D	273	LEU	N-CA-C	5.29	117.04	111.28
4	D	425	ARG	N-CA-C	5.29	117.04	111.28
4	D	366	PHE	N-CA-C	-5.28	105.52	111.28
4	D	426	ALA	O-C-N	-5.28	115.77	122.27
2	A	2125	G	C2'-C3'-O3'	5.28	121.61	113.70
4	D	152	ARG	N-CA-C	5.28	118.67	111.39
5	F	57	GLN	CB-CG-CD	-5.28	103.63	112.60
8	I	47	GLU	O-C-N	5.28	127.71	122.12
4	D	362	LYS	CB-CG-CD	5.27	123.43	111.30
2	A	2191	A	C3'-C2'-C1'	5.27	106.57	101.30
8	I	102	TRP	CE2-CD2-CE3	5.27	124.07	118.80
4	D	56	ASP	CA-CB-CG	-5.26	107.34	112.60
4	D	203	ARG	N-CA-CB	-5.26	102.38	110.01
8	I	69	ARG	N-CA-C	5.26	117.24	109.50
2	A	2137	U	P-O5'-C5'	5.26	128.79	120.90
2	A	2182	U	O3'-P-O5'	-5.26	96.11	104.00
6	G	37	MET	O-C-N	-5.26	117.04	123.30
4	D	360	ALA	N-CA-CB	-5.26	101.66	110.39
4	D	48	LEU	CA-C-O	5.26	126.34	120.82
6	G	49	LEU	CA-C-N	5.26	127.32	120.28
6	G	49	LEU	C-N-CA	5.26	127.32	120.28
8	I	26	VAL	N-CA-C	5.25	120.26	109.34
2	A	2128	G	O4'-C1'-N9	5.25	116.08	108.20
5	F	48	LEU	CA-C-N	5.25	125.70	120.98
5	F	48	LEU	C-N-CA	5.25	125.70	120.98
8	I	91	ARG	NE-CZ-NH1	5.25	126.75	121.50
2	A	1855	U	C4'-C3'-O3'	-5.25	105.13	113.00
2	A	1867	G	C4'-C3'-C2'	-5.25	97.35	102.60
6	G	118	ALA	N-CA-C	-5.25	105.16	112.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	167	ALA	O-C-N	5.25	128.13	122.15
6	G	63	LYS	CA-C-N	5.24	126.39	119.84
6	G	63	LYS	C-N-CA	5.24	126.39	119.84
4	D	60	GLU	CB-CG-CD	5.24	121.51	112.60
5	F	19	LYS	O-C-N	-5.24	117.41	123.33
8	I	137	ARG	NE-CZ-NH2	-5.24	114.49	119.20
4	D	457	LYS	N-CA-C	5.24	116.68	110.97
2	A	2188	U	C4'-C3'-C2'	5.23	107.83	102.60
2	A	1873	G	P-O5'-C5'	5.22	128.73	120.90
4	D	366	PHE	CA-C-O	5.22	126.09	120.55
8	I	50	ALA	CA-C-N	5.22	129.34	120.88
8	I	50	ALA	C-N-CA	5.22	129.34	120.88
4	D	81	ASN	N-CA-CB	-5.22	102.58	109.78
2	A	1881	C	O4'-C1'-N1	5.22	116.33	108.50
3	E	44	A	O4'-C1'-N9	5.22	116.33	108.50
2	A	2112	G	O3'-P-O5'	-5.22	96.18	104.00
4	D	435	GLY	O-C-N	-5.21	116.97	122.13
1	B	1299	A	O4'-C1'-C2'	5.21	111.01	105.80
7	H	45	HIS	CB-CG-ND1	5.21	130.51	122.70
5	F	184	LYS	O-C-N	-5.21	116.22	122.15
4	D	501	ARG	N-CA-CB	-5.20	102.47	110.01
2	A	1847	A	C2'-C3'-O3'	5.20	117.30	109.50
3	E	15	G	C1'-O4'-C4'	5.20	115.10	109.90
4	D	191	ASN	OD1-CG-ND2	-5.20	117.40	122.60
2	A	1847	A	O4'-C1'-C2'	5.20	111.00	105.80
3	E	56	U	P-O5'-C5'	5.20	128.69	120.90
5	F	195	ALA	O-C-N	5.20	127.42	122.07
6	G	67	THR	N-CA-C	5.19	117.56	110.55
4	D	125	GLN	N-CA-CB	-5.19	102.50	110.12
4	D	138	HIS	N-CA-CB	5.19	119.87	111.21
2	A	1851	U	O4'-C1'-N1	5.18	116.26	108.50
2	A	2190	G	O4'-C1'-N9	5.18	116.27	108.50
5	F	117	SER	CA-C-O	-5.17	115.33	120.66
4	D	139	ASN	O-C-N	5.17	127.60	122.12
1	B	1300	G	C5'-C4'-C3'	-5.17	107.44	115.20
5	F	38	PHE	CA-CB-CG	-5.17	108.63	113.80
2	A	2122	U	O4'-C1'-N1	5.17	116.25	108.50
2	A	2147	A	C2'-C3'-O3'	5.17	117.25	109.50
4	D	77	GLU	CA-C-N	5.17	126.30	119.84
4	D	77	GLU	C-N-CA	5.17	126.30	119.84
4	D	39	GLY	O-C-N	-5.17	119.04	123.43
8	I	95	ARG	NH1-CZ-NH2	-5.16	112.59	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1851	U	C3'-C2'-C1'	-5.16	96.14	101.30
6	G	147	ARG	CG-CD-NE	-5.16	100.65	112.00
4	D	160	ILE	CA-C-O	5.16	126.26	120.64
2	A	1834	U	O3'-P-O5'	-5.16	96.27	104.00
4	D	75	PRO	CA-C-N	5.16	128.15	120.31
4	D	75	PRO	C-N-CA	5.16	128.15	120.31
6	G	150	GLY	N-CA-C	-5.15	106.61	112.79
4	D	372	GLN	CA-C-O	5.15	125.91	119.78
4	D	149	ASP	N-CA-CB	-5.15	102.54	110.16
6	G	172	PHE	O-C-N	-5.15	115.58	122.94
2	A	1905	C	C3'-C2'-C1'	5.15	106.45	101.30
5	F	102	ASP	N-CA-C	5.15	119.43	113.20
2	A	2181	U	O4'-C1'-N1	5.14	116.22	108.50
2	A	2139	U	O4'-C1'-N1	5.14	116.21	108.50
4	D	454	HIS	ND1-CE1-NE2	5.14	113.54	108.40
4	D	492	GLY	N-CA-C	-5.14	106.37	111.56
1	B	1291	U	O3'-P-O5'	-5.14	96.29	104.00
8	I	116	ALA	CA-C-O	5.14	125.85	119.79
5	F	7	ARG	N-CA-C	5.14	117.62	111.71
5	F	41	SER	CA-C-N	-5.14	116.47	123.10
5	F	41	SER	C-N-CA	-5.14	116.47	123.10
5	F	161	VAL	N-CA-CB	5.14	118.32	111.64
8	I	129	ASN	CA-C-O	-5.13	115.64	121.65
4	D	277	ARG	CB-CA-C	5.13	119.31	110.79
2	A	2119	A	C4'-C3'-O3'	5.13	117.09	109.40
3	E	14	A	P-O3'-C3'	-5.13	112.51	120.20
3	E	63	C	O3'-P-O5'	-5.13	96.31	104.00
5	F	126	GLN	O-C-N	-5.12	116.31	122.15
3	E	8	U	C4'-C3'-O3'	-5.12	105.31	113.00
4	D	306	ASN	CA-C-N	5.12	127.15	120.28
4	D	306	ASN	C-N-CA	5.12	127.15	120.28
6	G	167	ALA	N-CA-C	5.12	116.94	111.36
2	A	2164	C	C5'-C4'-O4'	-5.12	102.12	109.80
3	E	35	C	O4'-C1'-C2'	-5.12	102.48	107.60
5	F	78	PHE	CA-CB-CG	-5.12	108.68	113.80
2	A	2170	A	C4'-C3'-O3'	-5.12	105.33	113.00
3	E	30	G	P-O5'-C5'	5.12	128.57	120.90
4	D	442	VAL	CA-C-N	5.11	126.78	120.34
4	D	442	VAL	C-N-CA	5.11	126.78	120.34
7	H	18	HIS	CA-CB-CG	5.11	118.91	113.80
1	B	1297	G	P-O5'-C5'	-5.11	113.24	120.90
4	D	5	VAL	N-CA-C	-5.11	105.15	112.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	89	ALA	CA-C-O	5.11	126.02	120.55
7	H	50	GLU	CA-C-O	5.11	127.81	120.51
2	A	1841	U	P-O5'-C5'	5.11	128.56	120.90
2	A	2129	C	C5'-C4'-C3'	5.10	122.84	115.20
6	G	11	VAL	N-CA-C	5.10	115.82	110.62
6	G	133	GLU	CB-CA-C	5.10	118.30	110.14
1	B	1291	U	C3'-C2'-C1'	5.09	106.39	101.30
1	B	1297	G	C4'-C3'-C2'	5.09	107.69	102.60
4	D	375	PRO	O-C-N	-5.08	117.44	122.98
8	I	127	ALA	CA-C-N	5.08	130.61	121.66
8	I	127	ALA	C-N-CA	5.08	130.61	121.66
1	B	1290	G	C1'-C2'-O2'	5.08	116.02	108.40
2	A	2173	A	C4'-C3'-C2'	5.08	107.68	102.60
4	D	206	HIS	CE1-NE2-CD2	-5.08	103.92	109.00
3	E	53	G	O5'-C5'-C4'	5.08	119.31	111.70
2	A	1858	A	C4'-C3'-C2'	-5.07	97.53	102.60
6	G	167	ALA	CA-C-N	5.07	127.38	120.54
6	G	167	ALA	C-N-CA	5.07	127.38	120.54
3	E	9	G	O3'-P-O5'	-5.07	96.40	104.00
4	D	212	VAL	N-CA-C	5.07	115.42	108.12
5	F	77	VAL	CA-C-O	5.07	126.05	120.48
8	I	147	ASN	N-CA-C	5.07	119.22	113.19
1	B	1239	A	O4'-C4'-C3'	-5.06	101.04	106.10
5	F	209	ILE	N-CA-C	-5.06	101.18	108.42
4	D	364	THR	CA-C-N	5.06	127.48	120.29
4	D	364	THR	C-N-CA	5.06	127.48	120.29
2	A	2152	G	P-O5'-C5'	5.06	128.49	120.90
3	E	70	C	C1'-C2'-O2'	5.06	115.99	108.40
3	E	74	A	P-O3'-C3'	5.06	127.79	120.20
5	F	164	ARG	NE-CZ-NH2	5.05	123.75	119.20
1	B	1300	G	C3'-C2'-O2'	-5.05	107.02	114.60
3	E	31	G	C5'-C4'-C3'	-5.05	108.42	116.00
4	D	56	ASP	O-C-N	-5.05	117.31	123.27
2	A	1884	G	O4'-C1'-N9	5.05	115.78	108.20
4	D	294	PHE	CA-CB-CG	5.05	118.85	113.80
4	D	394	PHE	N-CA-CB	5.05	118.02	109.94
6	G	137	PHE	N-CA-C	5.05	117.05	110.08
8	I	13	PRO	CA-C-N	5.05	130.08	121.35
8	I	13	PRO	C-N-CA	5.05	130.08	121.35
5	F	7	ARG	CG-CD-NE	-5.04	100.91	112.00
6	G	75	GLY	N-CA-C	5.04	120.22	114.67
3	E	42	C	C4'-C3'-C2'	-5.04	97.56	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	71	ILE	CA-C-N	-5.04	117.41	122.20
4	D	71	ILE	C-N-CA	-5.04	117.41	122.20
2	A	2171	A	C1'-O4'-C4'	-5.04	104.66	109.70
7	H	28	THR	O-C-N	-5.04	116.26	122.20
2	A	1860	G	P-O5'-C5'	-5.04	113.35	120.90
4	D	540	ALA	N-CA-C	5.04	117.50	111.71
4	D	133	GLN	O-C-N	-5.03	116.78	122.12
8	I	91	ARG	NH1-CZ-NH2	5.03	125.84	119.30
2	A	1860	G	C4'-C3'-C2'	-5.03	97.57	102.60
3	E	52	C	O3'-P-O5'	5.03	111.55	104.00
4	D	370	SER	CA-C-O	5.03	125.36	119.28
5	F	139	ASN	CB-CA-C	5.03	117.91	109.32
2	A	1868	C	C3'-C2'-C1'	-5.02	96.28	101.30
4	D	9	HIS	CA-C-O	5.02	125.67	120.40
4	D	133	GLN	N-CA-CB	-5.02	102.74	110.12
4	D	531	GLU	CA-C-O	5.02	125.87	120.55
5	F	165	ASN	O-C-N	-5.02	117.29	122.96
8	I	113	LYS	N-CA-C	5.01	116.56	111.14
2	A	2147	A	P-O3'-C3'	5.01	127.72	120.20
4	D	41	ASN	CA-CB-CG	5.01	117.61	112.60
5	F	51	ASP	N-CA-C	-5.01	105.90	112.41
5	F	212	VAL	CB-CA-C	5.01	117.84	110.98
4	D	66	GLN	CG-CD-NE2	5.01	123.91	116.40
8	I	130	LYS	CA-C-N	5.01	131.22	121.41
8	I	130	LYS	C-N-CA	5.01	131.22	121.41
2	A	2101	A	O3'-P-O5'	-5.00	96.49	104.00
4	D	172	ALA	CA-C-O	5.00	125.86	120.55
2	A	1890	A	P-O3'-C3'	-5.00	112.69	120.20
7	H	7	LYS	CA-C-O	5.00	125.71	120.36

There are no chirality outliers.

All (178) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	1835	G	Sidechain
2	A	1838	C	Sidechain
2	A	1839	G	Sidechain
2	A	1840	G	Sidechain
2	A	1842	G	Sidechain
2	A	1843	C	Sidechain
2	A	1845	G	Sidechain
2	A	1846	G	Sidechain

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Mol	Chain	Res	Type	Group
2	A	1850	G	Sidechain
2	A	1857	G	Sidechain
2	A	1858	A	Sidechain
2	A	1859	U	Sidechain
2	A	1862	G	Sidechain
2	A	1863	G	Sidechain
2	A	1865	U	Sidechain
2	A	1868	C	Sidechain
2	A	1869	G	Sidechain
2	A	1874	C	Sidechain
2	A	1876	A	Sidechain
2	A	1878	G	Sidechain
2	A	1882	U	Sidechain
2	A	1884	G	Sidechain
2	A	1886	U	Sidechain
2	A	1888	G	Sidechain
2	A	1889	A	Sidechain
2	A	1891	G	Sidechain
2	A	1894	C	Sidechain
2	A	1895	C	Sidechain
2	A	1896	G	Sidechain
2	A	1900	A	Sidechain
2	A	2094	A	Sidechain
2	A	2095	A	Sidechain
2	A	2102	G	Sidechain
2	A	2103	C	Sidechain
2	A	2104	C	Sidechain
2	A	2106	U	Sidechain
2	A	2109	U	Sidechain
2	A	2110	G	Sidechain
2	A	2111	U	Sidechain
2	A	2112	G	Sidechain
2	A	2114	A	Sidechain
2	A	2115	G	Sidechain
2	A	2116	G	Sidechain
2	A	2120	G	Sidechain
2	A	2123	G	Sidechain
2	A	2124	G	Sidechain
2	A	2125	G	Sidechain
2	A	2127	G	Sidechain
2	A	2128	G	Sidechain
2	A	2129	C	Sidechain

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Mol	Chain	Res	Type	Group
2	A	2130	U	Sidechain
2	A	2132	U	Sidechain
2	A	2133	G	Sidechain
2	A	2135	A	Sidechain
2	A	2136	G	Sidechain
2	A	2137	U	Sidechain
2	A	2138	G	Sidechain
2	A	2141	G	Sidechain
2	A	2144	G	Sidechain
2	A	2147	A	Sidechain
2	A	2148	G	Sidechain
2	A	2152	G	Sidechain
2	A	2153	C	Sidechain
2	A	2154	A	Sidechain
2	A	2156	G	Sidechain
2	A	2157	G	Sidechain
2	A	2158	A	Sidechain
2	A	2159	G	Sidechain
2	A	2160	C	Sidechain
2	A	2161	C	Sidechain
2	A	2164	C	Sidechain
2	A	2165	C	Sidechain
2	A	2166	U	Sidechain
2	A	2168	G	Sidechain
2	A	2176	A	Sidechain
2	A	2177	C	Sidechain
2	A	2179	C	Sidechain
2	A	2184	A	Sidechain
2	A	2186	G	Sidechain
2	A	2187	U	Sidechain
2	A	2189	U	Sidechain
2	A	2190	G	Sidechain
2	A	2191	A	Sidechain
2	A	2192	U	Sidechain
1	B	1239	A	Sidechain
1	B	1242	G	Sidechain
1	B	1243	C	Sidechain
1	B	1290	G	Sidechain
1	B	1295	U	Sidechain
1	B	1296	C	Sidechain
1	B	1301	U	Sidechain
1	B	1302	C	Sidechain

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Mol	Chain	Res	Type	Group
1	B	1304	G	Sidechain
1	B	1332	A	Sidechain
1	B	1334	G	Sidechain
1	B	1336	C	Sidechain
4	D	111	TYR	Sidechain
4	D	181	PRO	Peptide
4	D	186	LEU	Peptide
4	D	19	ARG	Sidechain
4	D	225	VAL	Peptide
4	D	254	ARG	Sidechain
4	D	290	ARG	Sidechain
4	D	293	ARG	Sidechain
4	D	316	GLY	Peptide
4	D	318	ARG	Sidechain
4	D	330	ARG	Sidechain
4	D	333	TYR	Sidechain
4	D	336	ARG	Sidechain
4	D	366	PHE	Sidechain
4	D	392	ASP	Peptide
4	D	395	ARG	Sidechain
4	D	427	TYR	Sidechain
4	D	441	ARG	Sidechain
4	D	481	ARG	Sidechain
4	D	503	PHE	Sidechain
4	D	508	ALA	Peptide
4	D	530	TYR	Sidechain
4	D	550	TYR	Sidechain
3	E	1	C	Sidechain
3	E	11	A	Sidechain
3	E	12	G	Sidechain
3	E	13	C	Sidechain
3	E	15	G	Sidechain
3	E	18	U	Sidechain
3	E	19	G	Sidechain
3	E	22	A	Sidechain
3	E	23	G	Sidechain
3	E	28	U	Sidechain
3	E	29	C	Sidechain
3	E	3	C	Sidechain
3	E	30	G	Sidechain
3	E	35	C	Sidechain
3	E	36	A	Sidechain

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Mol	Chain	Res	Type	Group
3	E	37	U	Sidechain
3	E	38	A	Sidechain
3	E	4	G	Sidechain
3	E	40	C	Sidechain
3	E	42	C	Sidechain
3	E	44	A	Sidechain
3	E	47	G	Sidechain
3	E	5	G	Sidechain
3	E	53	G	Sidechain
3	E	59	A	Sidechain
3	E	60	A	Sidechain
3	E	61	U	Sidechain
3	E	63	C	Sidechain
3	E	64	G	Sidechain
3	E	7	G	Sidechain
3	E	73	A	Sidechain
3	E	74	A	Sidechain
3	E	8	U	Sidechain
3	E	9	G	Sidechain
5	F	12	ARG	Sidechain
5	F	124	VAL	Peptide
5	F	134	ARG	Sidechain
5	F	162	ARG	Sidechain
5	F	163	TYR	Sidechain
5	F	164	ARG	Sidechain
5	F	203	GLN	Peptide
5	F	35	THR	Peptide
5	F	7	ARG	Sidechain
6	G	124	ARG	Sidechain
6	G	149	ARG	Sidechain
6	G	177	ARG	Sidechain
6	G	6	TYR	Sidechain
6	G	76	PHE	Sidechain
6	G	91	ARG	Sidechain
7	H	20	TYR	Sidechain
7	H	27	ARG	Sidechain
7	H	48	TYR	Sidechain
7	H	5	ARG	Sidechain
8	I	101	ARG	Sidechain
8	I	4	ARG	Sidechain
8	I	52	ARG	Sidechain
8	I	69	ARG	Sidechain

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Mol	Chain	Res	Type	Group
8	I	78	ARG	Sidechain
8	I	95	ARG	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	B	687	0	342	24	0
2	A	3731	0	1828	68	0
3	E	1640	0	827	29	0
4	D	4393	0	4377	340	0
5	F	1733	0	1824	153	0
6	G	1420	0	1460	10	0
7	H	410	0	440	1	0
8	I	1182	0	1240	126	0
All	All	15196	0	12338	429	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 16.

All (429) 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:B:1240:U:C4	8:I:31:VAL:HG12	1.20	1.68
4:D:108:TYR:HA	5:F:118:PRO:CB	1.17	1.59
4:D:108:TYR:CA	5:F:118:PRO:HB2	1.27	1.57
4:D:108:TYR:CE2	5:F:121:MET:HB3	1.34	1.57
4:D:523:PHE:CD1	8:I:130:LYS:HB2	1.37	1.57
2:A:2169:A:C2	4:D:141:ASN:HB2	1.40	1.55
4:D:111:TYR:CD1	5:F:147:PRO:HA	1.42	1.53
4:D:536:ARG:NH1	8:I:137:ARG:NH2	1.65	1.44
4:D:133:GLN:HG2	5:F:60:ARG:CD	1.44	1.42
1:B:1240:U:C4	8:I:31:VAL:CG1	2.11	1.34
4:D:536:ARG:NH1	8:I:137:ARG:HH22	0.83	1.31
4:D:108:TYR:C	5:F:118:PRO:HB2	1.57	1.29
2:A:2113:U:C4'	4:D:147:ALA:HA	1.63	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:108:TYR:CA	5:F:118:PRO:CB	1.94	1.28
4:D:108:TYR:HB3	5:F:118:PRO:O	1.29	1.28
4:D:322:LYS:CG	8:I:113:LYS:HZ3	1.45	1.27
4:D:523:PHE:HD1	8:I:130:LYS:CB	1.45	1.27
1:B:1240:U:C1'	8:I:37:THR:HG21	1.64	1.27
4:D:129:GLU:OE1	5:F:143:GLY:HA3	1.18	1.27
4:D:108:TYR:OH	5:F:121:MET:HG2	1.34	1.26
4:D:533:TYR:HB2	8:I:129:ASN:O	1.08	1.26
2:A:2169:A:H2	4:D:141:ASN:CB	1.49	1.23
4:D:322:LYS:HG3	8:I:113:LYS:NZ	1.51	1.23
4:D:536:ARG:HH12	8:I:137:ARG:NH2	1.24	1.22
4:D:108:TYR:CE2	5:F:121:MET:CB	2.22	1.21
4:D:133:GLN:CG	5:F:60:ARG:HD2	1.70	1.21
4:D:140:LEU:HD21	5:F:129:GLN:CG	1.69	1.20
4:D:133:GLN:CG	5:F:60:ARG:CD	2.20	1.19
4:D:111:TYR:CB	5:F:118:PRO:HG3	1.73	1.18
4:D:125:GLN:NE2	5:F:144:THR:HG23	1.59	1.18
4:D:108:TYR:CE1	5:F:145:VAL:HG11	1.79	1.17
4:D:111:TYR:HB2	5:F:118:PRO:CG	1.74	1.17
4:D:532:GLU:HG3	8:I:138:GLU:OE1	1.47	1.14
2:A:2113:U:H1'	4:D:146:ARG:HG3	1.30	1.14
4:D:536:ARG:HH22	8:I:137:ARG:NH1	1.43	1.13
4:D:412:LEU:HD21	6:G:46:LYS:H	1.07	1.13
2:A:2113:U:C5'	4:D:147:ALA:HA	1.80	1.12
4:D:533:TYR:CB	8:I:129:ASN:O	1.96	1.12
4:D:108:TYR:HB3	5:F:118:PRO:C	1.74	1.11
2:A:2169:A:C2	4:D:141:ASN:CB	2.25	1.11
4:D:137:GLY:HA2	5:F:129:GLN:HE21	1.16	1.11
4:D:130:GLU:HB3	5:F:55:SER:HB3	1.22	1.10
4:D:523:PHE:HB2	8:I:130:LYS:HD2	1.31	1.10
1:B:1240:U:C2	8:I:37:THR:CG2	2.35	1.10
2:A:2113:U:C2	4:D:143:GLN:OE1	2.03	1.10
4:D:111:TYR:CE1	5:F:147:PRO:HA	1.86	1.09
4:D:111:TYR:CD1	5:F:147:PRO:CA	2.36	1.08
2:A:2113:U:H1'	4:D:146:ARG:CG	1.84	1.08
2:A:2113:U:C1'	4:D:146:ARG:HG3	1.81	1.08
1:B:1240:U:O2	8:I:37:THR:CG2	2.03	1.07
2:A:2113:U:C6	4:D:143:GLN:NE2	2.21	1.07
4:D:536:ARG:NH2	8:I:137:ARG:HH12	1.50	1.06
3:E:3:C:H1'	4:D:277:ARG:NH2	1.72	1.05
4:D:129:GLU:OE1	5:F:143:GLY:CA	2.03	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:140:LEU:CD2	5:F:129:GLN:HG3	1.87	1.04
1:B:1240:U:O4	8:I:31:VAL:HG12	1.58	1.03
3:E:17:C:OP2	3:E:18:U:C5	2.11	1.03
4:D:111:TYR:HE1	5:F:147:PRO:HB3	1.23	1.02
1:B:1240:U:C5	8:I:31:VAL:CG1	2.43	1.02
2:A:2113:U:C5	4:D:143:GLN:NE2	2.28	1.02
4:D:111:TYR:CE1	5:F:147:PRO:CA	2.43	1.01
4:D:133:GLN:OE1	5:F:141:LYS:HB3	1.60	1.01
4:D:536:ARG:CZ	8:I:137:ARG:HH22	1.73	1.01
1:B:1240:U:C5	8:I:31:VAL:HG12	1.96	1.01
4:D:108:TYR:O	5:F:118:PRO:HB2	1.59	1.00
4:D:111:TYR:CE2	5:F:145:VAL:HG23	1.96	0.99
4:D:108:TYR:CG	5:F:118:PRO:HA	1.97	0.99
4:D:108:TYR:HA	5:F:118:PRO:HB3	0.99	0.98
4:D:523:PHE:CD1	8:I:130:LYS:CB	2.28	0.98
3:E:3:C:C1'	4:D:277:ARG:HH21	1.77	0.98
4:D:108:TYR:CB	5:F:118:PRO:O	2.10	0.97
2:A:2113:U:H5'	4:D:147:ALA:HA	1.43	0.97
4:D:412:LEU:HD21	6:G:46:LYS:N	1.80	0.97
4:D:108:TYR:CE1	5:F:145:VAL:CG1	2.48	0.97
4:D:140:LEU:HD21	5:F:129:GLN:HG3	0.99	0.96
2:A:2169:A:N3	4:D:141:ASN:OD1	1.97	0.96
4:D:141:ASN:OD1	5:F:127:LEU:HD13	1.65	0.95
1:B:1240:U:C2	8:I:37:THR:HG23	2.00	0.95
4:D:111:TYR:HB2	5:F:118:PRO:HG3	0.95	0.94
2:A:2113:U:C2'	4:D:146:ARG:HG3	1.97	0.94
2:A:2113:U:O2'	4:D:146:ARG:HG3	1.67	0.94
2:A:2113:U:H4'	4:D:147:ALA:HA	1.47	0.93
4:D:118:PHE:CE2	5:F:148:ASN:ND2	2.37	0.93
4:D:529:GLU:CD	8:I:135:LYS:HD2	1.93	0.93
1:B:1240:U:H1'	8:I:37:THR:HG21	1.49	0.92
5:F:60:ARG:HH12	5:F:164:ARG:NE	1.67	0.92
4:D:533:TYR:HD1	4:D:533:TYR:O	1.53	0.91
2:A:2169:A:C2	4:D:141:ASN:OD1	2.23	0.91
4:D:111:TYR:HE2	5:F:145:VAL:HG23	1.36	0.90
4:D:108:TYR:CZ	5:F:121:MET:HB3	2.07	0.90
4:D:322:LYS:CG	8:I:113:LYS:NZ	2.21	0.90
4:D:108:TYR:HE2	5:F:121:MET:HB3	1.32	0.89
4:D:130:GLU:HB3	5:F:55:SER:CB	2.03	0.89
4:D:130:GLU:O	5:F:55:SER:OG	1.90	0.89
4:D:111:TYR:HD1	5:F:147:PRO:HA	1.21	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:118:PHE:HD1	4:D:118:PHE:H	1.21	0.89
3:E:72:C:O2'	4:D:278:GLN:O	1.89	0.88
4:D:125:GLN:CD	5:F:144:THR:HA	1.99	0.87
2:A:2113:U:C4'	4:D:147:ALA:CA	2.51	0.87
8:I:125:ASP:OD1	8:I:130:LYS:HE2	1.75	0.87
2:A:2113:U:O2	4:D:146:ARG:NE	2.08	0.87
4:D:524:GLU:CB	8:I:110:ARG:NE	2.37	0.87
4:D:111:TYR:HB3	5:F:83:ASN:ND2	1.90	0.86
1:B:1240:U:O4'	8:I:37:THR:HG21	1.75	0.86
4:D:133:GLN:OE1	5:F:141:LYS:CB	2.23	0.86
4:D:524:GLU:OE1	8:I:110:ARG:HG3	1.75	0.86
1:B:1240:U:O2	8:I:37:THR:HG22	1.75	0.86
2:A:1907:G:N2	3:E:12:G:O3'	2.08	0.86
4:D:108:TYR:CD1	5:F:118:PRO:HA	2.10	0.85
4:D:108:TYR:CD1	5:F:145:VAL:HG21	2.11	0.85
4:D:523:PHE:CE1	8:I:130:LYS:HB2	2.11	0.85
4:D:111:TYR:CE1	5:F:147:PRO:HB3	2.12	0.85
4:D:533:TYR:HD1	4:D:533:TYR:C	1.86	0.84
4:D:533:TYR:CD1	4:D:533:TYR:C	2.51	0.84
4:D:524:GLU:CG	8:I:110:ARG:NE	2.41	0.84
4:D:118:PHE:HE2	5:F:148:ASN:ND2	1.74	0.84
5:F:60:ARG:NH1	5:F:164:ARG:CD	2.41	0.84
4:D:140:LEU:HD21	5:F:129:GLN:CB	2.08	0.83
4:D:528:THR:HB	8:I:142:ARG:CZ	2.08	0.83
4:D:524:GLU:CG	8:I:110:ARG:HE	1.92	0.83
3:E:72:C:C5'	4:D:278:GLN:HE21	1.92	0.82
4:D:129:GLU:CD	5:F:143:GLY:HA3	2.03	0.82
4:D:533:TYR:HD2	8:I:130:LYS:HB3	1.43	0.82
4:D:526:ASN:HB2	4:D:529:GLU:OE2	1.79	0.82
4:D:322:LYS:CB	8:I:113:LYS:NZ	2.42	0.82
4:D:108:TYR:CZ	5:F:121:MET:HG2	2.14	0.82
3:E:17:C:OP2	3:E:18:U:C6	2.33	0.82
4:D:528:THR:HB	8:I:142:ARG:NH2	1.94	0.82
2:A:2113:U:H5'	4:D:147:ALA:CA	2.10	0.81
4:D:529:GLU:CD	8:I:135:LYS:CG	2.53	0.81
4:D:108:TYR:O	5:F:118:PRO:CB	2.29	0.81
4:D:529:GLU:CD	8:I:135:LYS:CD	2.53	0.81
4:D:533:TYR:CE2	8:I:130:LYS:HD3	2.16	0.81
4:D:111:TYR:HE1	5:F:147:PRO:CB	1.94	0.81
4:D:133:GLN:HG2	5:F:60:ARG:HD3	1.62	0.81
4:D:524:GLU:HG2	8:I:110:ARG:CD	2.09	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:526:ASN:N	4:D:529:GLU:OE2	2.13	0.80
4:D:108:TYR:CB	5:F:118:PRO:CB	2.59	0.80
4:D:108:TYR:CB	5:F:118:PRO:HB2	2.11	0.80
4:D:111:TYR:CE1	5:F:147:PRO:CB	2.66	0.79
4:D:529:GLU:CG	8:I:135:LYS:HG3	2.13	0.79
5:F:60:ARG:HH12	5:F:164:ARG:CZ	1.96	0.78
4:D:108:TYR:CB	5:F:118:PRO:C	2.57	0.78
1:B:1240:U:N1	8:I:37:THR:HG21	1.97	0.78
4:D:108:TYR:CG	5:F:118:PRO:CA	2.65	0.78
4:D:532:GLU:CG	8:I:138:GLU:OE1	2.29	0.78
4:D:133:GLN:CD	5:F:60:ARG:HD3	2.09	0.78
4:D:524:GLU:CD	8:I:110:ARG:HG3	2.09	0.78
3:E:3:C:C2'	4:D:277:ARG:HH21	1.95	0.78
4:D:322:LYS:HG3	8:I:113:LYS:HZ3	0.66	0.78
4:D:108:TYR:CD2	5:F:121:MET:HB3	2.17	0.77
2:A:1907:G:H21	3:E:13:C:P	2.07	0.77
4:D:111:TYR:HB3	5:F:83:ASN:HD21	1.47	0.77
4:D:529:GLU:CD	8:I:135:LYS:HG3	2.10	0.77
4:D:108:TYR:CE2	5:F:121:MET:CG	2.68	0.77
4:D:533:TYR:HE2	8:I:130:LYS:HD3	1.50	0.77
2:A:2169:A:C2	4:D:141:ASN:CG	2.64	0.76
4:D:412:LEU:CD2	6:G:46:LYS:H	1.94	0.76
4:D:105:ASP:OD2	5:F:122:ARG:HB3	1.86	0.76
4:D:108:TYR:CZ	5:F:121:MET:CB	2.66	0.76
4:D:533:TYR:HB2	8:I:129:ASN:C	2.08	0.75
4:D:133:GLN:HG2	5:F:60:ARG:HD2	0.77	0.75
4:D:529:GLU:OE1	8:I:135:LYS:HD2	1.87	0.75
4:D:524:GLU:HB3	8:I:110:ARG:CZ	2.16	0.74
4:D:108:TYR:CB	5:F:118:PRO:CA	2.64	0.74
4:D:524:GLU:CB	8:I:110:ARG:CZ	2.64	0.74
4:D:108:TYR:CZ	5:F:145:VAL:HG11	2.20	0.74
4:D:133:GLN:CG	5:F:60:ARG:HD3	2.16	0.73
4:D:529:GLU:OE1	8:I:135:LYS:HB2	1.88	0.73
4:D:524:GLU:HG2	8:I:110:ARG:HG3	1.71	0.73
4:D:138:HIS:CE1	4:D:140:LEU:HD23	2.24	0.73
4:D:412:LEU:HD21	6:G:46:LYS:HB2	1.71	0.73
4:D:532:GLU:HB3	8:I:138:GLU:CD	2.13	0.73
4:D:529:GLU:HG2	8:I:135:LYS:HG3	1.71	0.73
4:D:529:GLU:OE2	8:I:135:LYS:NZ	2.18	0.72
4:D:322:LYS:HB3	8:I:113:LYS:HZ1	1.55	0.72
4:D:141:ASN:OD1	5:F:127:LEU:CD1	2.38	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:536:ARG:HH12	8:I:137:ARG:CZ	2.01	0.72
4:D:137:GLY:HA2	5:F:129:GLN:NE2	1.98	0.72
5:F:60:ARG:NH1	5:F:164:ARG:NE	2.36	0.72
4:D:510:HIS:NE2	4:D:524:GLU:CD	2.48	0.72
4:D:322:LYS:CB	8:I:113:LYS:HZ1	2.00	0.72
4:D:108:TYR:OH	5:F:121:MET:CG	2.28	0.71
4:D:111:TYR:CD2	5:F:118:PRO:HG3	2.25	0.71
4:D:125:GLN:HE22	5:F:144:THR:HG23	1.51	0.70
4:D:108:TYR:CD2	5:F:118:PRO:O	2.45	0.70
4:D:111:TYR:CG	5:F:118:PRO:HG3	2.26	0.70
2:A:2113:U:O2'	4:D:146:ARG:CG	2.40	0.70
1:B:1240:U:C2	8:I:37:THR:HG21	2.16	0.69
2:A:2113:U:H5''	4:D:150:ALA:HB3	1.74	0.69
4:D:524:GLU:HG2	8:I:110:ARG:CG	2.23	0.69
4:D:536:ARG:HH12	8:I:137:ARG:HH22	0.79	0.69
4:D:108:TYR:O	5:F:118:PRO:CG	2.40	0.69
3:E:3:C:O2	4:D:277:ARG:NH2	2.27	0.68
3:E:3:C:C1'	4:D:277:ARG:NH2	2.40	0.68
3:E:17:C:OP2	3:E:18:U:H5	1.70	0.68
4:D:105:ASP:OD2	5:F:122:ARG:CB	2.42	0.68
4:D:524:GLU:HG2	8:I:110:ARG:NE	2.07	0.68
4:D:510:HIS:HE2	4:D:524:GLU:CD	2.02	0.67
1:B:1240:U:N1	8:I:37:THR:CG2	2.55	0.67
4:D:108:TYR:CZ	5:F:121:MET:CG	2.78	0.67
4:D:524:GLU:CG	8:I:110:ARG:HG3	2.24	0.66
1:B:1240:U:O2	8:I:34:LYS:HB2	1.95	0.66
2:A:2113:U:O4'	4:D:147:ALA:CA	2.44	0.66
4:D:526:ASN:CB	4:D:529:GLU:OE2	2.44	0.66
1:B:1240:U:N3	8:I:31:VAL:HG12	2.00	0.66
3:E:3:C:H1'	4:D:277:ARG:HH22	1.58	0.66
4:D:133:GLN:HE22	5:F:141:LYS:HD3	1.61	0.65
5:F:60:ARG:NH1	5:F:164:ARG:CG	2.59	0.65
4:D:133:GLN:HE22	5:F:141:LYS:CD	2.09	0.65
4:D:322:LYS:HE3	8:I:112:ASP:C	2.22	0.65
4:D:524:GLU:CD	8:I:110:ARG:HE	2.03	0.65
4:D:524:GLU:HB2	8:I:110:ARG:NH2	2.12	0.65
4:D:108:TYR:HD1	5:F:145:VAL:HG21	1.57	0.65
4:D:322:LYS:HD2	8:I:113:LYS:HE2	1.79	0.65
2:A:1907:G:N2	3:E:13:C:OP1	2.27	0.65
3:E:54:G:H2'	3:E:55:U:C6	2.32	0.65
4:D:524:GLU:CB	8:I:110:ARG:HE	2.06	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:532:GLU:CB	8:I:138:GLU:CD	2.71	0.64
2:A:2113:U:O4'	4:D:147:ALA:HB2	1.97	0.64
3:E:17:C:P	3:E:18:U:H5	2.21	0.64
4:D:322:LYS:HG3	8:I:113:LYS:CE	2.28	0.64
1:B:1240:U:C1'	8:I:37:THR:CG2	2.58	0.63
4:D:108:TYR:HB3	5:F:118:PRO:CA	2.28	0.63
2:A:2113:U:H1'	4:D:146:ARG:HG2	1.78	0.63
4:D:130:GLU:CB	5:F:55:SER:HB3	2.13	0.63
2:A:2113:U:O4'	4:D:147:ALA:HA	1.98	0.62
4:D:108:TYR:CG	5:F:118:PRO:O	2.52	0.62
4:D:108:TYR:O	5:F:118:PRO:HG2	1.99	0.62
4:D:118:PHE:HD1	4:D:118:PHE:N	1.93	0.62
4:D:536:ARG:CZ	8:I:138:GLU:OE2	2.47	0.62
2:A:2113:U:C2	4:D:143:GLN:CD	2.78	0.62
2:A:2113:U:O2	4:D:146:ARG:CZ	2.48	0.62
2:A:2113:U:N3	4:D:143:GLN:OE1	2.32	0.62
4:D:108:TYR:CA	5:F:118:PRO:HB3	1.94	0.61
4:D:192:HIS:H	4:D:499:HIS:CE1	2.17	0.61
4:D:108:TYR:CE1	5:F:145:VAL:HG21	2.35	0.61
5:F:60:ARG:NH1	5:F:164:ARG:HD2	2.14	0.61
3:E:72:C:H4'	4:D:278:GLN:HG3	1.82	0.61
4:D:137:GLY:CA	5:F:129:GLN:HE21	2.02	0.61
4:D:510:HIS:CD2	4:D:524:GLU:CD	2.78	0.61
1:B:1240:U:O4'	8:I:37:THR:CG2	2.47	0.61
4:D:101:LEU:HD22	5:F:126:GLN:HE21	1.66	0.61
4:D:133:GLN:CD	5:F:60:ARG:CD	2.70	0.61
4:D:533:TYR:HD2	8:I:130:LYS:CB	2.13	0.61
4:D:525:GLY:HA3	4:D:529:GLU:OE1	2.00	0.60
2:A:2169:A:H2	4:D:141:ASN:HB2	0.60	0.60
4:D:111:TYR:CG	5:F:146:THR:O	2.55	0.60
4:D:133:GLN:OE1	5:F:60:ARG:HD3	2.02	0.60
5:F:60:ARG:NH1	5:F:164:ARG:HG2	2.17	0.59
4:D:118:PHE:N	4:D:118:PHE:CD1	2.65	0.59
4:D:129:GLU:OE1	5:F:144:THR:N	2.35	0.59
4:D:536:ARG:NH2	8:I:137:ARG:NH1	2.24	0.59
1:B:1240:U:H3	8:I:31:VAL:H	1.49	0.59
4:D:469:ASP:HA	4:D:497:ILE:HD12	1.85	0.59
2:A:2113:U:C5'	4:D:150:ALA:HB3	2.33	0.58
2:A:1907:G:N2	3:E:13:C:P	2.75	0.58
4:D:510:HIS:CD2	4:D:524:GLU:OE2	2.57	0.58
4:D:142:VAL:HG13	4:D:146:ARG:CZ	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:311:LEU:HG	4:D:312:PHE:H	1.69	0.57
5:F:60:ARG:HH12	5:F:164:ARG:CD	2.12	0.57
4:D:526:ASN:H	4:D:529:GLU:CD	2.11	0.57
2:A:1847:A:H62	2:A:1893:C:H41	1.52	0.57
2:A:2113:U:N1	4:D:143:GLN:NE2	2.52	0.57
4:D:111:TYR:HE2	5:F:145:VAL:CG2	2.14	0.57
8:I:125:ASP:OD1	8:I:130:LYS:CE	2.49	0.57
2:A:2113:U:H4'	4:D:147:ALA:CA	2.26	0.57
4:D:536:ARG:HH22	8:I:137:ARG:HH12	0.68	0.57
2:A:2113:U:O4'	4:D:147:ALA:CB	2.53	0.56
4:D:133:GLN:CG	5:F:60:ARG:NE	2.68	0.56
4:D:533:TYR:CD2	8:I:130:LYS:HB3	2.34	0.56
4:D:524:GLU:HB2	8:I:110:ARG:CZ	2.35	0.56
4:D:412:LEU:CD2	6:G:46:LYS:HB2	2.36	0.56
4:D:533:TYR:O	4:D:533:TYR:CD1	2.44	0.56
4:D:108:TYR:HE1	5:F:145:VAL:CG1	2.14	0.56
4:D:130:GLU:C	5:F:55:SER:HG	2.07	0.56
2:A:1843:C:H2'	2:A:1844:C:C6	2.41	0.55
3:E:3:C:O2	4:D:277:ARG:NE	2.38	0.55
4:D:125:GLN:CD	5:F:144:THR:HG23	2.27	0.55
3:E:3:C:O2	4:D:277:ARG:CZ	2.53	0.55
1:B:1240:U:C5	8:I:31:VAL:HG11	2.36	0.55
7:H:18:HIS:CE1	7:H:19:PHE:CZ	2.94	0.55
1:B:1240:U:O4'	8:I:37:THR:OG1	2.23	0.55
4:D:108:TYR:CE1	5:F:145:VAL:CG2	2.90	0.55
4:D:533:TYR:CA	8:I:129:ASN:O	2.53	0.54
4:D:524:GLU:HB2	8:I:110:ARG:HH21	1.70	0.54
4:D:129:GLU:OE1	5:F:143:GLY:C	2.50	0.54
4:D:529:GLU:HG2	8:I:135:LYS:CB	2.37	0.54
4:D:529:GLU:HG2	8:I:135:LYS:CG	2.37	0.54
4:D:108:TYR:HE2	5:F:121:MET:CB	1.94	0.53
4:D:524:GLU:HB3	8:I:110:ARG:NE	2.13	0.53
4:D:138:HIS:CD2	4:D:140:LEU:H	2.26	0.53
4:D:529:GLU:OE2	8:I:135:LYS:HD2	2.09	0.53
2:A:2113:U:H5''	4:D:150:ALA:CB	2.39	0.53
4:D:140:LEU:CD2	5:F:129:GLN:CB	2.83	0.53
5:F:166:ASP:CG	5:F:170:ILE:HG22	2.34	0.52
3:E:72:C:H5''	4:D:278:GLN:HE21	1.69	0.52
4:D:108:TYR:CE2	5:F:121:MET:HG2	2.43	0.52
2:A:2169:A:N3	4:D:141:ASN:CG	2.65	0.52
1:B:1240:U:O2	8:I:37:THR:HG21	1.98	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:125:GLN:CG	5:F:144:THR:HA	2.39	0.51
2:A:2113:U:O2	4:D:143:GLN:OE1	2.28	0.51
4:D:108:TYR:CD1	5:F:118:PRO:CA	2.88	0.51
4:D:118:PHE:CD2	5:F:148:ASN:ND2	2.78	0.51
3:E:3:C:C2'	4:D:277:ARG:NH2	2.69	0.51
4:D:118:PHE:CD2	5:F:147:PRO:HB2	2.46	0.51
4:D:125:GLN:HG2	4:D:126:GLY:N	2.26	0.50
4:D:368:MET:HB3	4:D:380:ILE:HD12	1.92	0.50
5:F:170:ILE:HG23	5:F:172:HIS:CE1	2.47	0.50
6:G:39:VAL:HG22	6:G:39:VAL:O	2.11	0.50
8:I:119:LEU:HD13	8:I:123:LEU:HG	1.94	0.50
3:E:72:C:O5'	4:D:278:GLN:NE2	2.45	0.50
2:A:2166:U:C5	2:A:2167:U:C4	3.00	0.49
4:D:111:TYR:HD2	5:F:118:PRO:HB3	1.78	0.49
4:D:97:VAL:HG21	4:D:135:HIS:CD2	2.47	0.49
4:D:322:LYS:CE	8:I:112:ASP:O	2.60	0.49
4:D:532:GLU:HB3	8:I:138:GLU:OE2	2.11	0.49
8:I:28:ILE:HG21	8:I:101:ARG:HA	1.93	0.49
4:D:111:TYR:HD2	5:F:118:PRO:CG	2.26	0.49
4:D:108:TYR:HE2	5:F:121:MET:CG	2.16	0.49
2:A:1843:C:H2'	2:A:1844:C:H6	1.79	0.48
2:A:2113:U:C5'	4:D:147:ALA:CA	2.69	0.48
2:A:2164:C:C2	2:A:2172:U:C5	3.02	0.48
3:E:72:C:H4'	4:D:278:GLN:CG	2.43	0.48
5:F:104:ILE:HD13	5:F:104:ILE:H	1.79	0.48
4:D:414:ILE:HB	6:G:44:ALA:HA	1.96	0.48
8:I:137:ARG:O	8:I:141:HIS:CD2	2.67	0.48
4:D:111:TYR:CD2	5:F:118:PRO:CG	2.96	0.47
4:D:111:TYR:CD1	5:F:146:THR:O	2.67	0.47
2:A:1878:G:C6	2:A:1879:C:C4	3.02	0.47
3:E:17:C:P	3:E:18:U:C5	3.01	0.47
3:E:72:C:H6	3:E:72:C:H5'	1.78	0.47
5:F:60:ARG:HH11	5:F:164:ARG:HD2	1.80	0.47
4:D:105:ASP:OD2	5:F:122:ARG:HD3	2.15	0.47
4:D:529:GLU:CG	8:I:135:LYS:CG	2.86	0.47
2:A:2107:G:C6	2:A:2183:A:C2	3.03	0.47
2:A:2115:G:H3'	2:A:2116:G:C5'	2.45	0.47
4:D:133:GLN:CD	5:F:60:ARG:HH11	2.23	0.47
4:D:111:TYR:CD2	5:F:146:THR:O	2.68	0.47
5:F:151:GLU:HA	5:F:154:LYS:HE3	1.97	0.47
4:D:125:GLN:HG3	5:F:144:THR:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1242:G:C6	1:B:1243:C:C4	3.03	0.46
4:D:412:LEU:CD2	6:G:46:LYS:N	2.63	0.46
4:D:523:PHE:HB2	8:I:130:LYS:CD	2.22	0.46
6:G:102:LEU:HA	6:G:106:ALA:HB3	1.97	0.46
2:A:2183:A:H2'	2:A:2184:A:C8	2.50	0.46
2:A:2107:G:C5	2:A:2183:A:C2	3.04	0.46
2:A:2155:U:C5	2:A:2156:G:C5	3.04	0.46
4:D:118:PHE:HB3	5:F:147:PRO:HB2	1.98	0.46
4:D:523:PHE:CE2	4:D:525:GLY:O	2.69	0.46
3:E:72:C:C4'	4:D:278:GLN:HE21	2.28	0.45
8:I:125:ASP:HB3	8:I:131:GLY:CA	2.45	0.45
3:E:72:C:C5'	4:D:278:GLN:NE2	2.72	0.45
4:D:322:LYS:HE2	8:I:112:ASP:O	2.16	0.45
4:D:125:GLN:OE1	5:F:144:THR:HA	2.15	0.45
4:D:524:GLU:CB	8:I:110:ARG:NH2	2.76	0.45
4:D:301:GLU:OE1	4:D:305:ARG:NH2	2.50	0.45
4:D:526:ASN:HB2	8:I:135:LYS:HZ3	1.81	0.45
4:D:311:LEU:HB2	4:D:482:ALA:HB1	1.98	0.45
5:F:60:ARG:NH2	5:F:165:ASN:O	2.50	0.45
4:D:511:ILE:HB	4:D:523:PHE:CD2	2.52	0.44
4:D:529:GLU:OE2	8:I:135:LYS:CD	2.65	0.44
4:D:533:TYR:CD2	8:I:130:LYS:HD3	2.52	0.44
4:D:130:GLU:C	5:F:55:SER:OG	2.59	0.44
4:D:325:GLU:OE1	8:I:113:LYS:HE3	2.17	0.44
4:D:368:MET:CB	4:D:380:ILE:HD12	2.48	0.44
4:D:277:ARG:HD3	4:D:277:ARG:C	2.43	0.44
4:D:510:HIS:HD2	4:D:524:GLU:OE2	1.99	0.44
4:D:526:ASN:N	4:D:529:GLU:CD	2.72	0.44
4:D:415:MET:HG3	4:D:424:SER:HB3	1.99	0.43
2:A:2113:U:C4	4:D:143:GLN:NE2	2.79	0.43
2:A:2120:G:N7	5:F:1:MET:HE3	2.32	0.43
8:I:129:ASN:HA	8:I:134:VAL:HG21	1.99	0.43
4:D:536:ARG:NH1	8:I:137:ARG:CZ	2.66	0.43
4:D:529:GLU:HG2	8:I:135:LYS:HA	2.00	0.43
2:A:2167:U:C4	2:A:2168:G:C5	3.07	0.43
4:D:262:GLU:CD	4:D:265:ARG:HH12	2.27	0.43
4:D:523:PHE:CD2	4:D:523:PHE:C	2.94	0.43
4:D:524:GLU:HB2	8:I:110:ARG:NE	2.27	0.43
4:D:322:LYS:HE3	8:I:112:ASP:CA	2.49	0.43
8:I:125:ASP:HB3	8:I:131:GLY:HA2	2.00	0.43
4:D:511:ILE:HB	4:D:523:PHE:HD2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2113:U:C2	4:D:143:GLN:NE2	2.87	0.42
4:D:528:THR:CB	8:I:142:ARG:NH2	2.77	0.42
5:F:104:ILE:H	5:F:104:ILE:CD1	2.32	0.42
4:D:76:GLN:HE21	4:D:187:ASP:CG	2.27	0.42
5:F:76:ALA:HB2	5:F:111:PHE:CE2	2.53	0.42
3:E:17:C:O5'	3:E:18:U:H5	2.03	0.42
2:A:2113:U:H4'	4:D:146:ARG:O	2.20	0.42
4:D:111:TYR:HB2	5:F:118:PRO:HG2	1.88	0.42
2:A:1885:A:O4'	4:D:4:PHE:HZ	2.03	0.42
4:D:510:HIS:NE2	4:D:524:GLU:OE1	2.36	0.42
2:A:2108:A:C2	2:A:2109:U:C5	3.08	0.42
4:D:322:LYS:CE	8:I:112:ASP:C	2.92	0.42
4:D:523:PHE:CB	8:I:130:LYS:HD2	2.23	0.42
4:D:533:TYR:HE1	4:D:537:THR:OG1	2.03	0.42
5:F:104:ILE:HD13	5:F:104:ILE:N	2.35	0.42
4:D:105:ASP:OD2	5:F:122:ARG:CD	2.67	0.42
4:D:523:PHE:CZ	4:D:530:TYR:HB2	2.54	0.42
4:D:532:GLU:CB	8:I:138:GLU:OE1	2.67	0.42
2:A:2096:C:H2'	2:A:2097:A:C8	2.55	0.41
2:A:2168:G:N2	2:A:2171:A:C8	2.88	0.41
4:D:133:GLN:OE1	5:F:141:LYS:CG	2.68	0.41
8:I:45:ALA:HA	8:I:120:ALA:HB2	2.01	0.41
2:A:2115:G:H3'	2:A:2116:G:H5''	2.01	0.41
4:D:322:LYS:HB3	8:I:113:LYS:NZ	2.22	0.41
4:D:529:GLU:CD	8:I:135:LYS:HB2	2.46	0.41
4:D:108:TYR:CE1	5:F:145:VAL:HG13	2.48	0.41
4:D:330:ARG:HB3	4:D:377:SER:HB3	2.03	0.41
2:A:1846:G:H3'	2:A:1847:A:H5''	2.02	0.41
2:A:1878:G:C5	2:A:1879:C:C5	3.08	0.41
4:D:133:GLN:OE1	5:F:141:LYS:CA	2.69	0.41
4:D:52:MET:HE2	4:D:52:MET:HB3	1.94	0.41
4:D:111:TYR:CE2	5:F:145:VAL:CG2	2.85	0.41
4:D:138:HIS:HE1	5:F:129:GLN:HB2	1.86	0.41
5:F:5:THR:O	5:F:9:ARG:HG3	2.20	0.41
5:F:47:ASN:HB2	5:F:211:LYS:O	2.21	0.41
8:I:68:VAL:HG11	8:I:103:ILE:HG13	2.02	0.41
2:A:1846:G:C6	2:A:1847:A:C6	3.09	0.41
4:D:73:TYR:HA	4:D:185:LEU:O	2.20	0.40
4:D:111:TYR:CE1	5:F:147:PRO:N	2.88	0.40
2:A:2113:U:H5'	4:D:147:ALA:O	2.21	0.40
5:F:60:ARG:CZ	5:F:164:ARG:HG2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:108:TYR:CZ	5:F:145:VAL:CG1	2.95	0.40
4:D:322:LYS:HE3	8:I:112:ASP:O	2.21	0.40
4:D:533:TYR:CD2	8:I:130:LYS:CG	3.04	0.40
4:D:412:LEU:HD21	6:G:46:LYS:CB	2.44	0.40
4:D:222:LEU:HD23	4:D:222:LEU:HA	1.87	0.40
4:D:354:ILE:HB	4:D:497:ILE:HG12	2.04	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	
4	D	552/561 (98%)	508 (92%)	27 (5%)	17 (3%)	3	22
5	F	232/234 (99%)	199 (86%)	23 (10%)	10 (4%)	2	17
6	G	176/178 (99%)	138 (78%)	26 (15%)	12 (7%)	1	11
7	H	48/50 (96%)	38 (79%)	9 (19%)	1 (2%)	5	30
8	I	149/151 (99%)	119 (80%)	23 (15%)	7 (5%)	2	16
All	All	1157/1174 (99%)	1002 (87%)	108 (9%)	47 (4%)	4	18

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	83	GLU
4	D	91	GLU
4	D	143	GLN
4	D	317	PRO
6	G	102	LEU
4	D	165	GLY
4	D	194	ASP
4	D	283	ARG

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Mol	Chain	Res	Type
4	D	295	GLU
5	F	4	LEU
5	F	167	LYS
5	F	203	GLN
6	G	78	ILE
6	G	84	ILE
6	G	100	GLU
6	G	104	THR
8	I	13	PRO
8	I	126	ALA
8	I	139	ASP
4	D	155	ASP
4	D	208	PHE
4	D	243	ASN
5	F	100	LEU
5	F	159	GLY
5	F	204	ALA
6	G	2	LYS
6	G	96	TRP
8	I	112	ASP
4	D	93	ALA
4	D	299	SER
5	F	110	ASN
6	G	51	ASN
6	G	101	ARG
7	H	4	ILE
8	I	52	ARG
4	D	181	PRO
6	G	125	GLY
8	I	10	LYS
6	G	4	HIS
6	G	39	VAL
4	D	142	VAL
4	D	279	GLY
8	I	28	ILE
4	D	225	VAL
5	F	73	VAL
5	F	147	PRO
5	F	233	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	
4	D	465/472 (98%)	441 (95%)	24 (5%)	21	42
5	F	181/181 (100%)	170 (94%)	11 (6%)	17	38
6	G	149/149 (100%)	145 (97%)	4 (3%)	39	61
7	H	45/45 (100%)	44 (98%)	1 (2%)	45	64
8	I	124/124 (100%)	117 (94%)	7 (6%)	19	40
All	All	964/971 (99%)	917 (95%)	47 (5%)	24	43

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	17	PRO
4	D	35	ILE
4	D	40	LEU
4	D	41	ASN
4	D	48	LEU
4	D	78	PRO
4	D	97	VAL
4	D	118	PHE
4	D	125	GLN
4	D	127	ARG
4	D	152	ARG
4	D	169	ARG
4	D	188	GLU
4	D	190	THR
4	D	203	ARG
4	D	246	SER
4	D	276	VAL
4	D	362	LYS
4	D	440	LYS
4	D	474	ASP
4	D	477	ILE
4	D	478	GLU
4	D	523	PHE

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Mol	Chain	Res	Type
4	D	533	TYR
5	F	1	MET
5	F	38	PHE
5	F	40	GLU
5	F	66	PRO
5	F	69	THR
5	F	75	VAL
5	F	104	ILE
5	F	113	VAL
5	F	161	VAL
5	F	186	LYS
5	F	224	VAL
6	G	43	ILE
6	G	64	PRO
6	G	84	ILE
6	G	135	ILE
7	H	46	VAL
8	I	8	GLN
8	I	26	VAL
8	I	49	LEU
8	I	51	GLN
8	I	72	VAL
8	I	93	VAL
8	I	130	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	20	HIS
4	D	76	GLN
4	D	125	GLN
4	D	138	HIS
4	D	206	HIS
4	D	257	GLN
4	D	278	GLN
4	D	328	ASN
4	D	438	GLN
4	D	499	HIS
5	F	67	HIS
5	F	126	GLN
5	F	129	GLN
5	F	148	ASN

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Mol	Chain	Res	Type
5	F	172	HIS
5	F	234	ASN
7	H	18	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	30/101 (29%)	12 (40%)	3 (10%)
2	A	172/360 (47%)	53 (30%)	9 (5%)
3	E	76/77 (98%)	19 (25%)	1 (1%)
All	All	278/538 (51%)	84 (30%)	13 (4%)

All (84) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	1238	A
1	B	1240	U
1	B	1243	C
1	B	1292	G
1	B	1293	C
1	B	1299	A
1	B	1300	G
1	B	1302	C
1	B	1304	G
1	B	1305	G
1	B	1335	U
1	B	1336	C
2	A	1846	G
2	A	1847	A
2	A	1848	A
2	A	1858	A
2	A	1859	U
2	A	1869	G
2	A	1870	C
2	A	1871	A
2	A	1872	A
2	A	1874	C
2	A	1884	G
2	A	1888	G
2	A	1903	G
2	A	1905	C

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Mol	Chain	Res	Type
2	A	1906	G
2	A	1907	G
2	A	2102	G
2	A	2104	C
2	A	2110	G
2	A	2111	U
2	A	2112	G
2	A	2113	U
2	A	2117	A
2	A	2119	A
2	A	2127	G
2	A	2130	U
2	A	2131	U
2	A	2132	U
2	A	2133	G
2	A	2134	A
2	A	2135	A
2	A	2136	G
2	A	2137	U
2	A	2144	G
2	A	2146	C
2	A	2147	A
2	A	2148	G
2	A	2149	U
2	A	2152	G
2	A	2153	C
2	A	2155	U
2	A	2157	G
2	A	2158	A
2	A	2159	G
2	A	2162	G
2	A	2164	C
2	A	2165	C
2	A	2167	U
2	A	2176	A
2	A	2179	C
2	A	2181	U
2	A	2187	U
2	A	2192	U
3	E	5	G
3	E	8	U
3	E	9	G

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Mol	Chain	Res	Type
3	E	13	C
3	E	17	C
3	E	18	U
3	E	19	G
3	E	20	G
3	E	21	U
3	E	22	A
3	E	48	U
3	E	49	C
3	E	50	G
3	E	54	G
3	E	72	C
3	E	74	A
3	E	75	C
3	E	76	C
3	E	77	A

All (13) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	B	1299	A
1	B	1332	A
1	B	1335	U
2	A	1871	A
2	A	2110	G
2	A	2126	A
2	A	2129	C
2	A	2152	G
2	A	2157	G
2	A	2158	A
2	A	2159	G
2	A	2172	U
3	E	9	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 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.

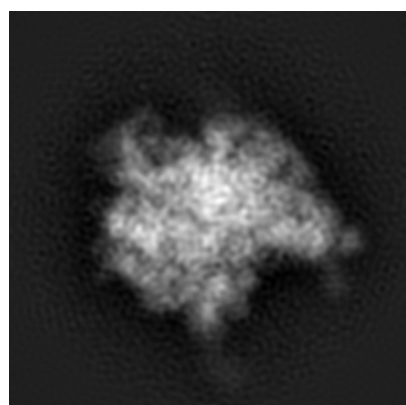
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5784. These allow visual inspection of the internal detail of the map and identification of artifacts.

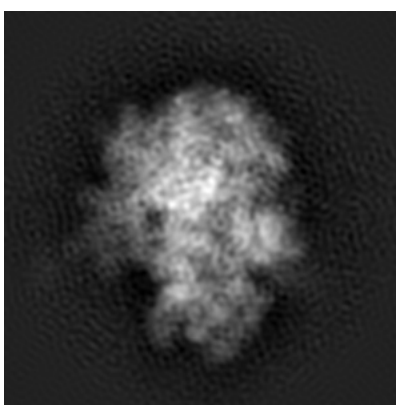
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

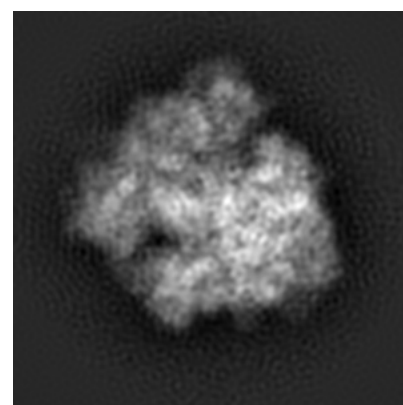
6.1.1 Primary map



X



Y

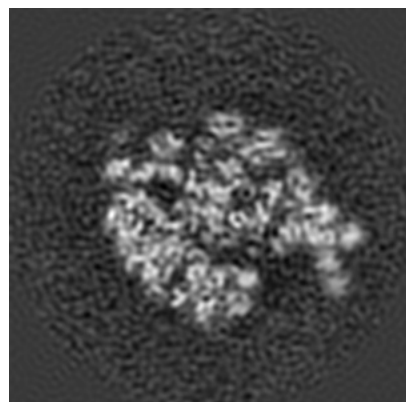


Z

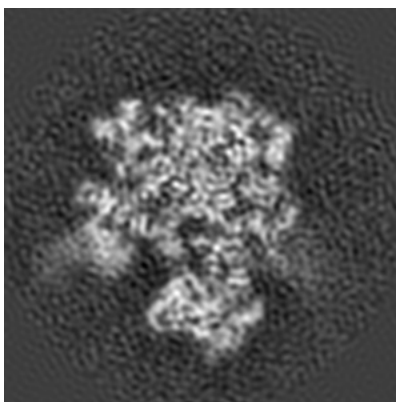
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

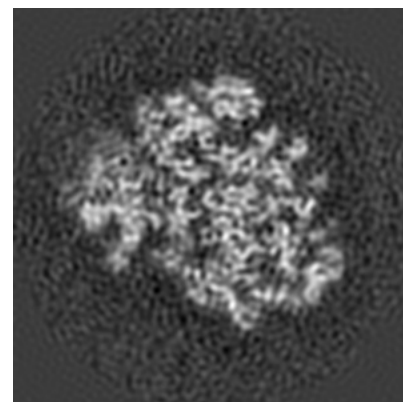
6.2.1 Primary map



X Index: 67



Y Index: 67

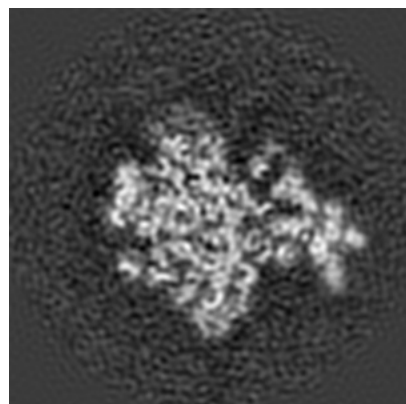


Z Index: 67

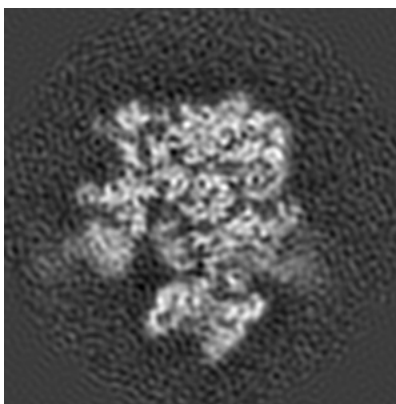
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

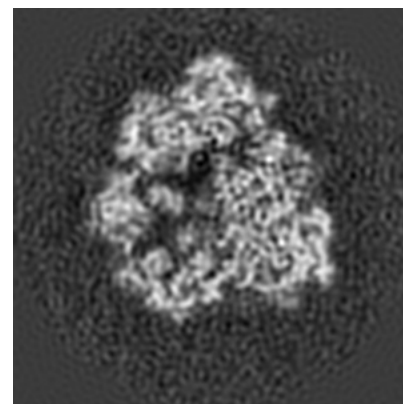
6.3.1 Primary map



X Index: 71



Y Index: 69

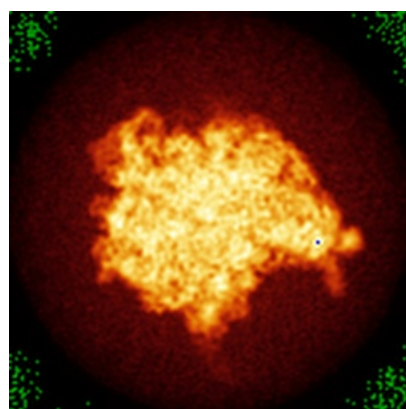


Z Index: 58

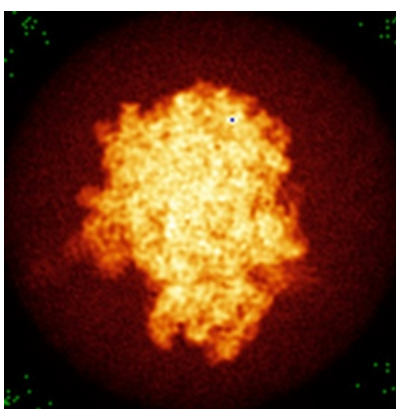
The images above show the largest variance slices of the map in three orthogonal directions.

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

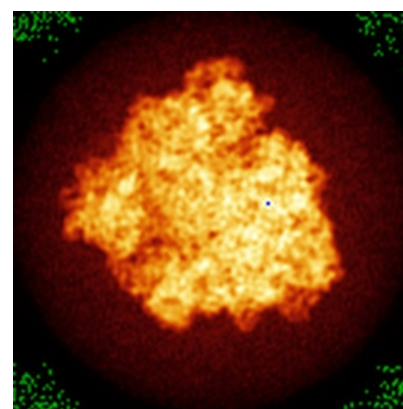
6.4.1 Primary map



X



Y



Z

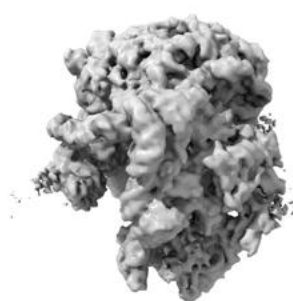
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

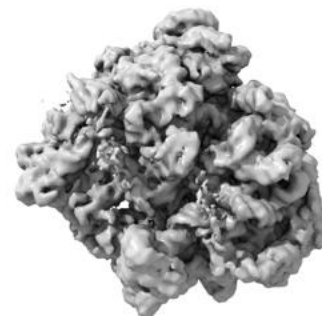
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 80.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

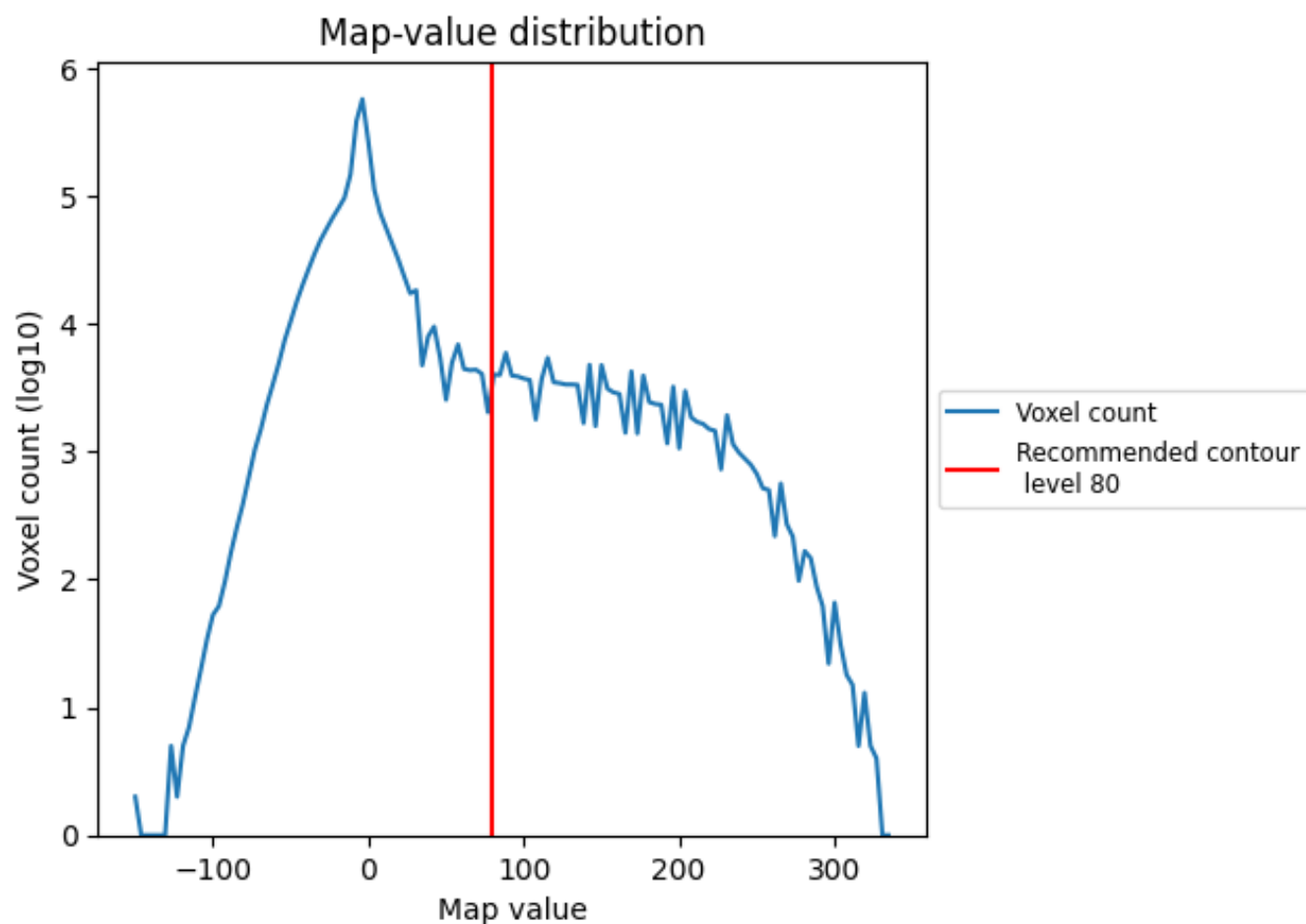
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

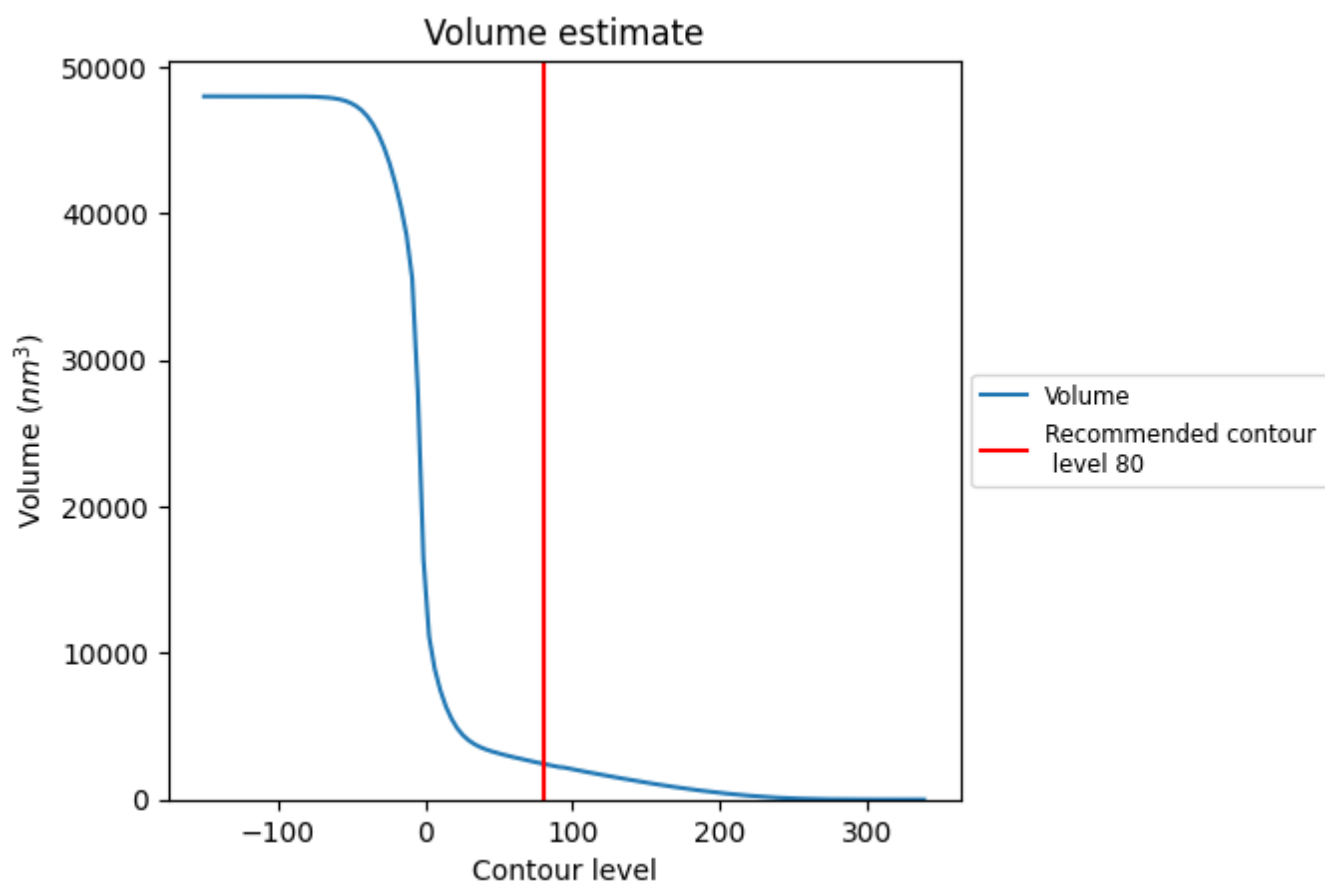
This section contains the results of statistical analysis of the map.

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.

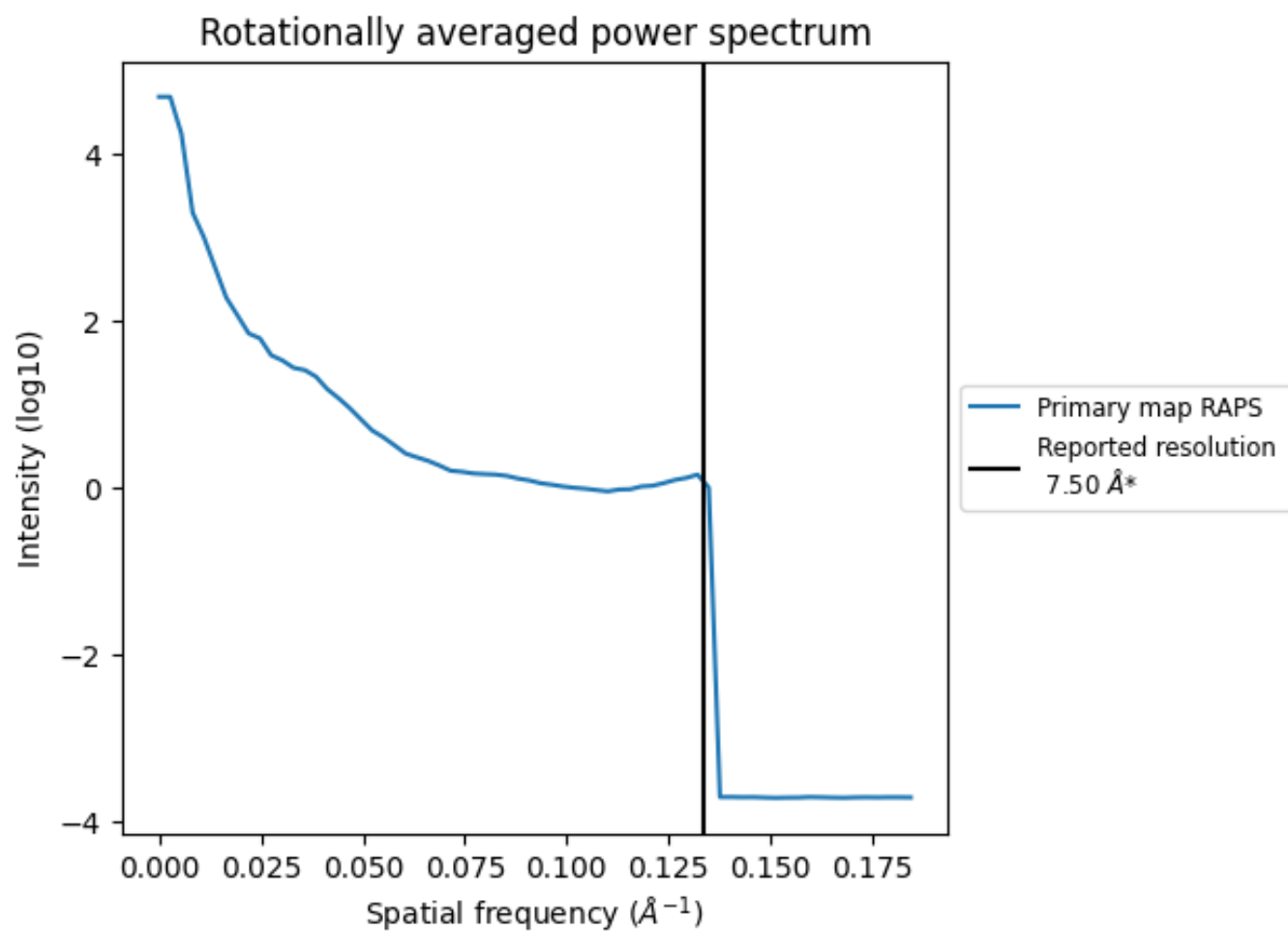
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2444 nm³; this corresponds to an approximate mass of 2208 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 0.133 Å⁻¹

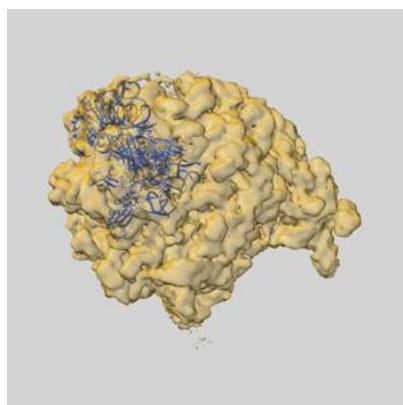
8 Fourier-Shell correlation ⓘ

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

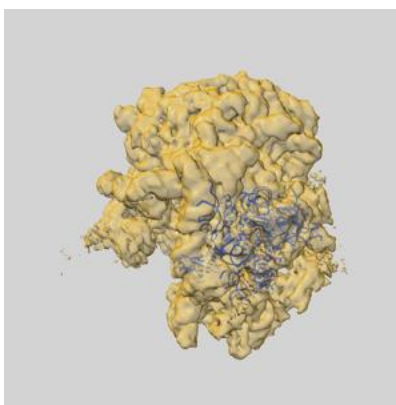
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-5784 and PDB model 3J5S. Per-residue inclusion information can be found in section 3 on page 6.

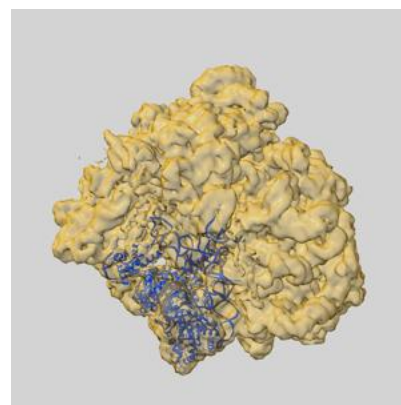
9.1 Map-model overlay [i](#)



X



Y



Z

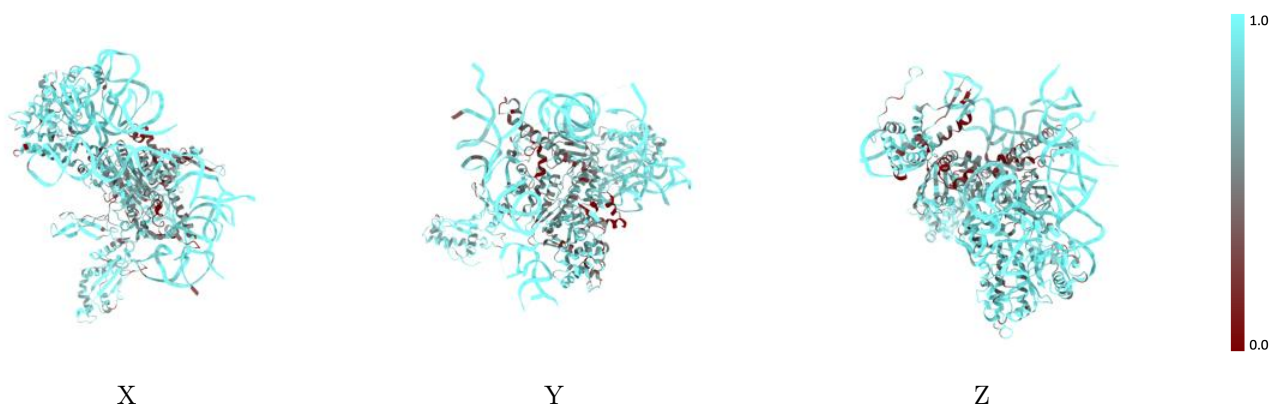
The images above show the 3D surface view of the map at the recommended contour level 80.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



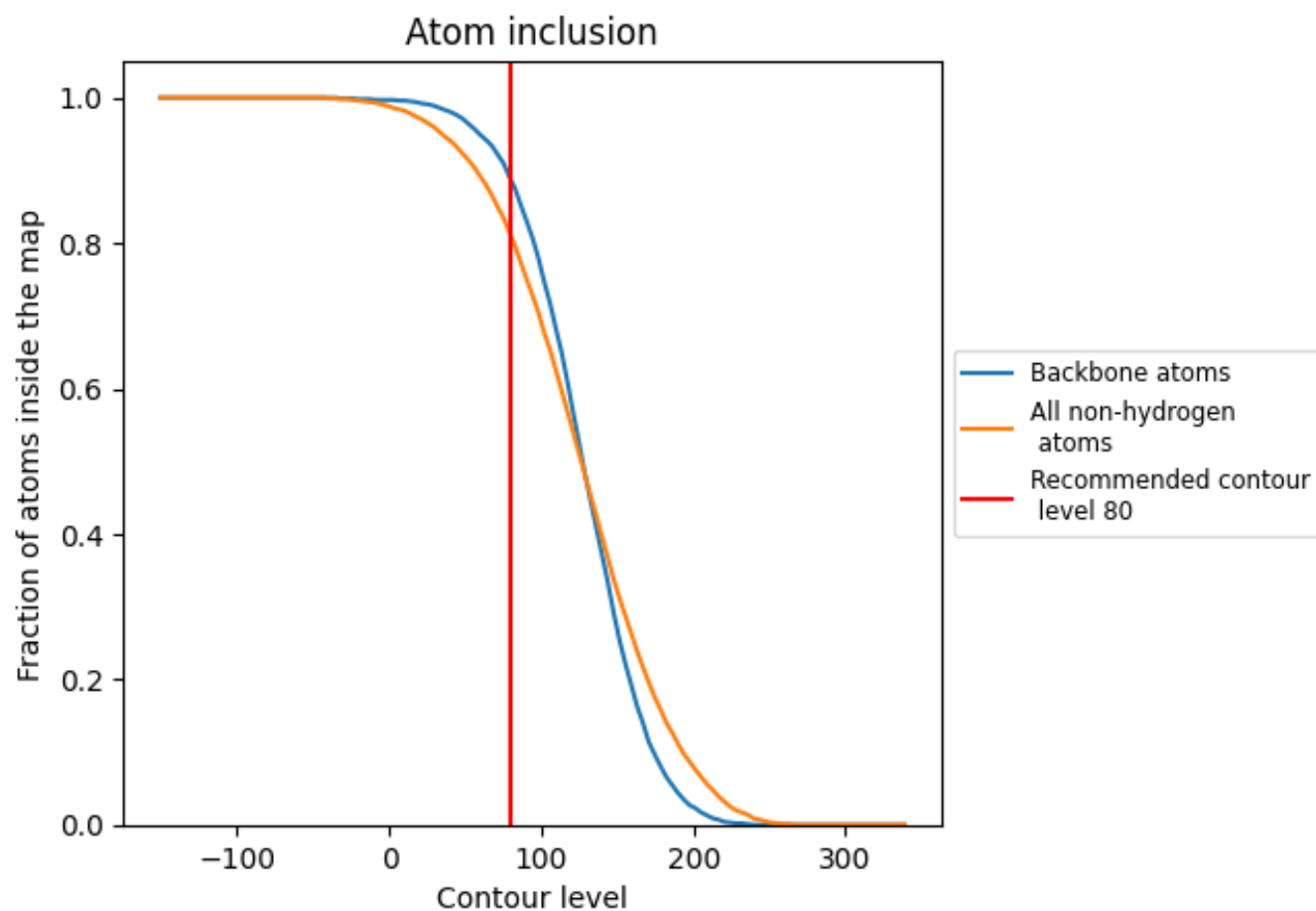
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (80).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 81% 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 (80) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8110	0.1220
A	0.9550	0.1600
B	0.9880	0.1690
D	0.6450	0.1120
E	0.8680	0.1700
F	0.8670	0.0700
G	0.8440	0.0980
H	0.7710	0.0940
I	0.6640	0.0650

1.0

0.0

<0.0