



Full wwPDB EM Validation Report ⓘ

Mar 17, 2026 – 03:14 PM UTC

PDB ID : 3J46 / pdb_00003j46
EMDB ID : EMD-5693
Title : Structure of the SecY protein translocation channel in action
Authors : Akey, C.W.; Park, E.; Menetret, J.F.; Gumbart, J.C.; Ludtke, S.J.; Li, W.;
Whynot, A.; Rapoport, T.A.
Deposited on : 2013-06-18
Resolution : 10.10 Å (reported)
Based on initial models : 3I8G, 3J01, 2I2P

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

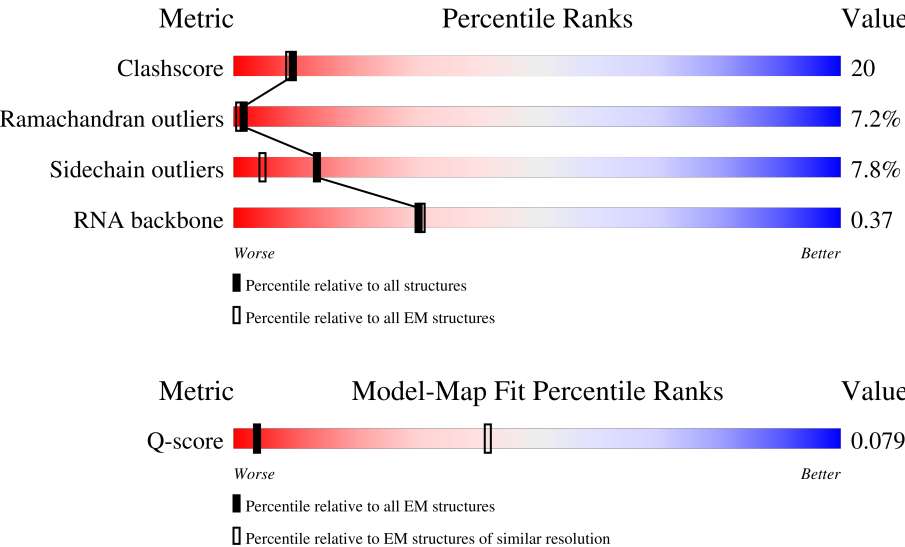
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance i

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

The reported resolution of this entry is 10.10 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	127 (9.60 - 10.60)

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

Mol	Chain	Length	Quality of chain
1	y	437	13% 28% 52% 15% 5%
2	E	56	23% 25% 54% 21%
3	G	67	10% 19% 58% 13% 9%

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Mol	Chain	Length	Quality of chain
4	n	101	
5	p	76	
6	a	76	
7	5	234	
8	T	100	
9	U	103	
10	Y	63	
11	1	63	
12	2	36	
13	3	44	
14	4	109	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 17478 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Protein translocase subunit SecY.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	y	437	Total	C	N	O	S	0	1
			3361	2220	554	569	18		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
y	5	ACE	-	acetylation	UNP P0AGA2
y	68	CYS	SER	engineered mutation	UNP P0AGA2
y	441	NH2	-	amidation	UNP P0AGA2

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	67	Total	C	N	O	S	0	1
			461	301	74	82	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	8	ACE	-	acetylation	UNP P0AG99
G	74	NH2	-	amidation	UNP P0AG99

- Molecule 4 is a protein called NC100.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	n	101	Total	C	N	O	S	0	0
			760	480	132	146	2		

- Molecule 5 is a RNA chain called P-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	p	76	Total	C	N	O	P	0	0
			1621	722	287	536	76		

- Molecule 6 is a RNA chain called A-tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	a	76	Total	C	N	O	P	S	0	0
			1626	729	290	531	75	1		

- Molecule 7 is a protein called 50S ribosomal protein L1.

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

- Molecule 8 is a protein called 50S ribosomal protein L23P.

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

- Molecule 9 is a protein called 50S ribosomal protein L24P.

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

- Molecule 10 is a protein called 50S ribosomal protein L29P.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	1	63	Total	C	N	O	P	0	0
			1350	603	245	439	63		

- Molecule 12 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	2	36	Total	C	N	O	P	0	0
			775	345	142	252	36		

- Molecule 13 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	3	44	Total	C	N	O	P	0	0
			948	423	180	301	44		

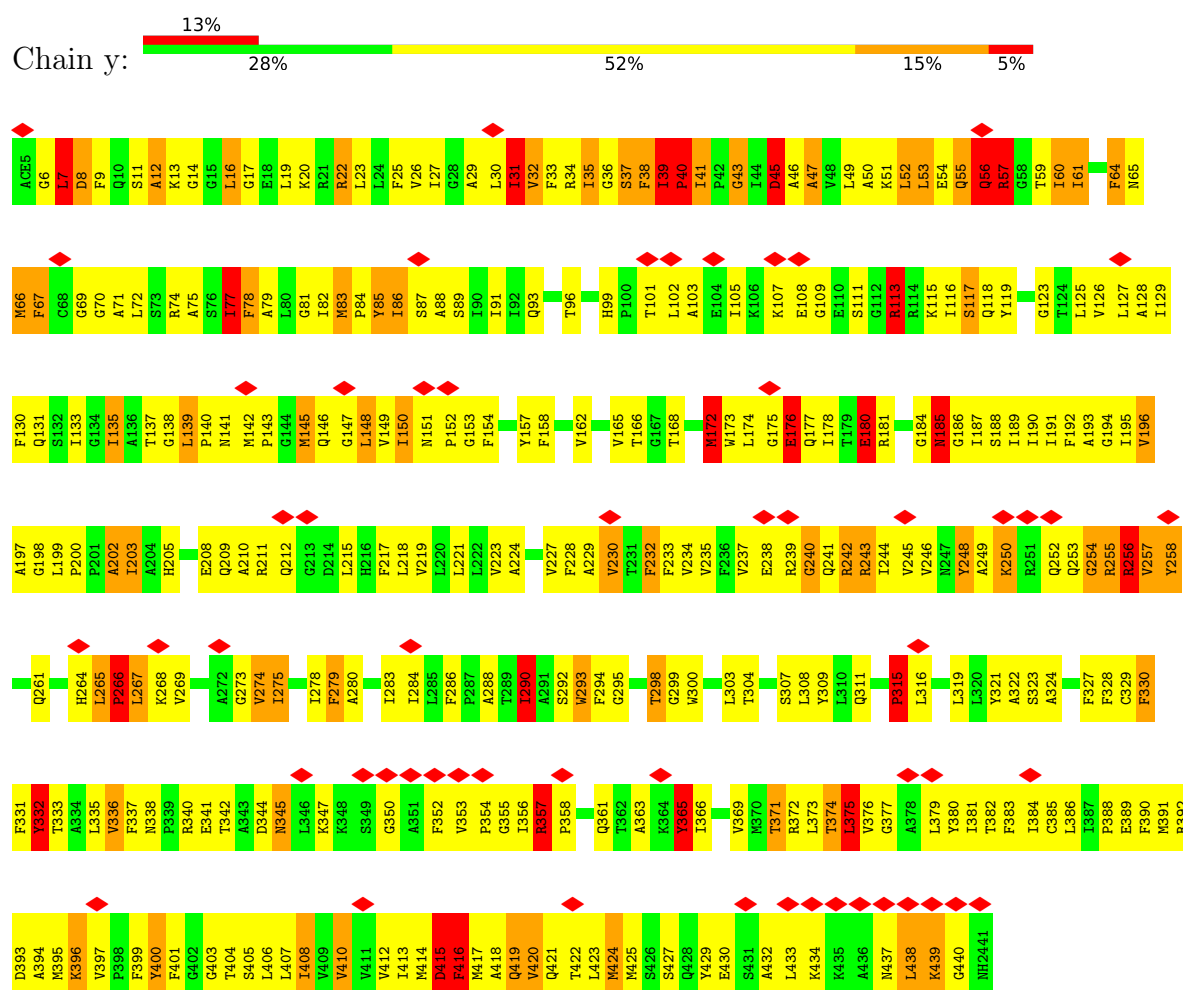
- Molecule 14 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	4	109	Total	C	N	O	P	0	0
			2325	1038	409	769	109		

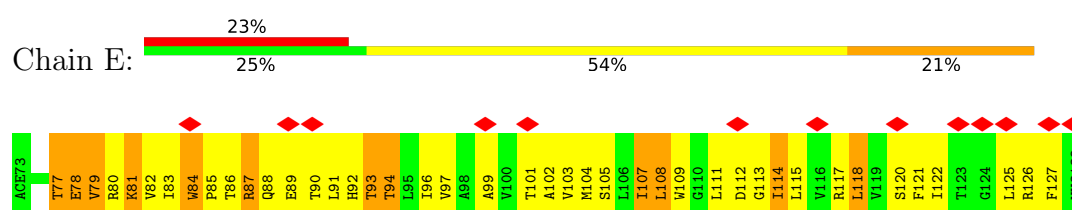
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

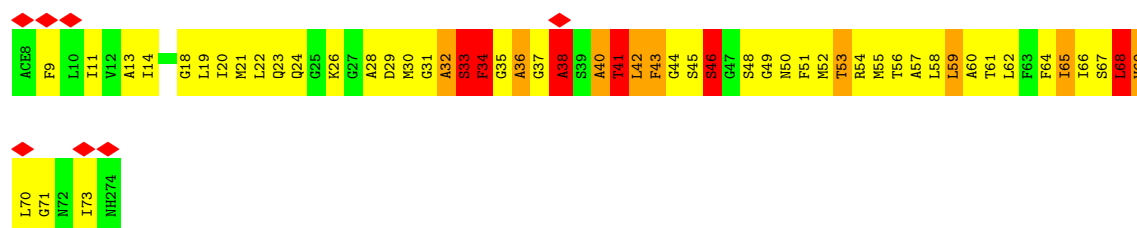
• Molecule 1: Protein translocase subunit SecY



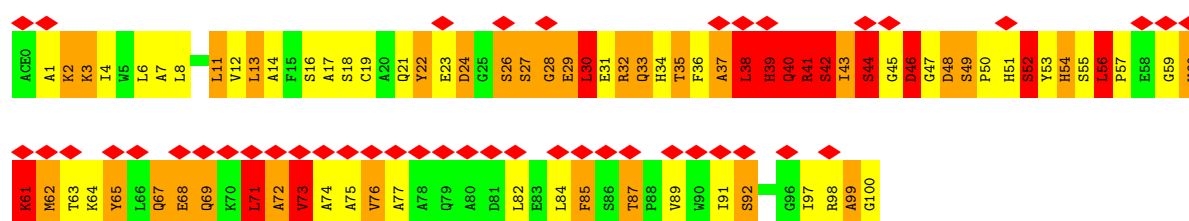
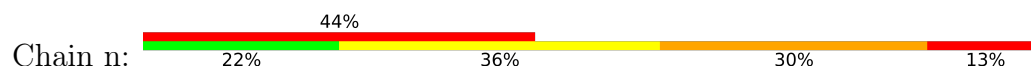
• Molecule 2: Preprotein translocase subunit SecE



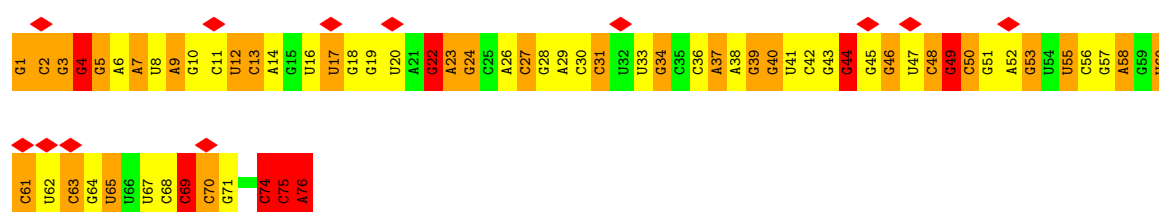
- Molecule 3: Protein-export membrane protein SecE



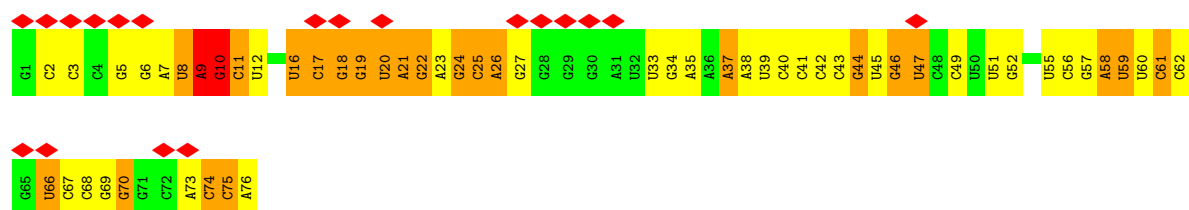
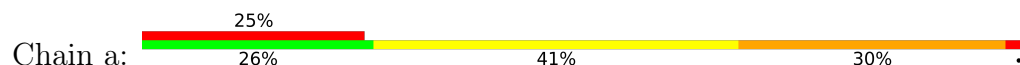
- Molecule 4: NC100



- Molecule 5: P-tRNA

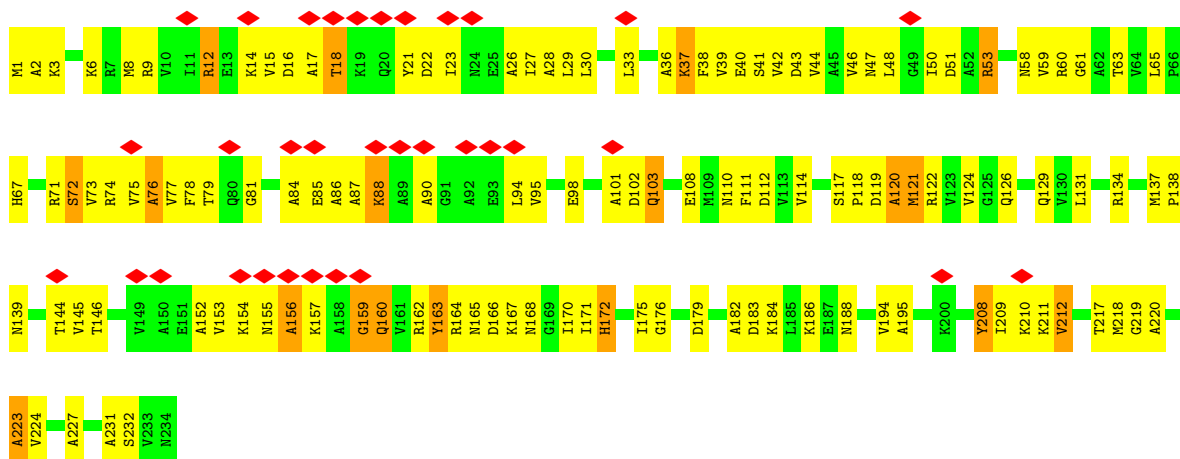


- Molecule 6: A-tRNA

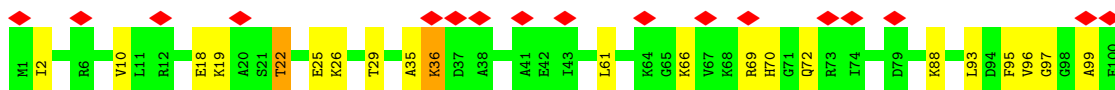
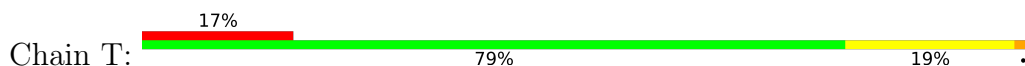


- Molecule 7: 50S ribosomal protein L1

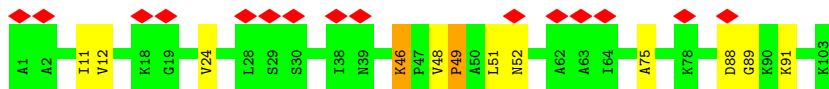
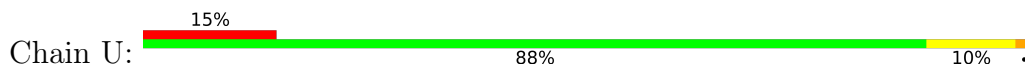




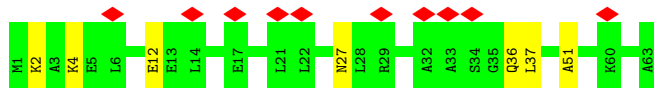
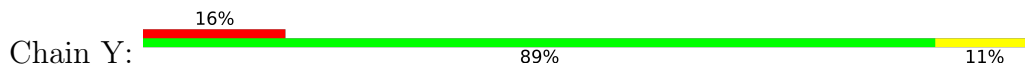
• Molecule 8: 50S ribosomal protein L23P



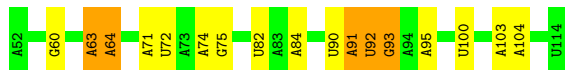
• Molecule 9: 50S ribosomal protein L24P



• Molecule 10: 50S ribosomal protein L29P



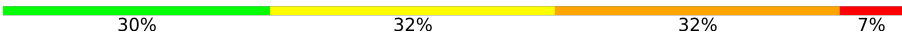
• Molecule 11: 23S ribosomal RNA



• Molecule 12: 23S ribosomal RNA



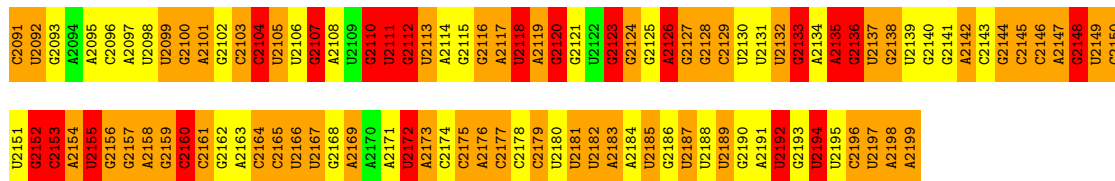
- Molecule 13: 23S ribosomal RNA

Chain 3:  30% 32% 32% 7%



- Molecule 14: 23S ribosomal RNA

Chain 4:  31% 47% 18%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	53000	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	per micrograph	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	160	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	42000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	3.245	Depositor
Minimum map value	-0.464	Depositor
Average map value	0.072	Depositor
Map value standard deviation	0.294	Depositor
Recommended contour level	0.8	Depositor
Map size ($\text{\AA}$)	407.03998, 407.03998, 407.03998	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	2.12, 2.12, 2.12	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	y	2.31	132/3434 (3.8%)	2.96	435/4657 (9.3%)
2	E	2.30	19/437 (4.3%)	3.24	64/596 (10.7%)
3	G	2.32	23/463 (5.0%)	3.02	71/622 (11.4%)
4	n	2.26	8/774 (1.0%)	1.95	30/1048 (2.9%)
5	p	1.91	24/1810 (1.3%)	1.82	53/2820 (1.9%)
6	a	0.33	0/1783	0.73	3/2776 (0.1%)
7	5	2.30	65/1748 (3.7%)	2.48	124/2355 (5.3%)
8	T	1.28	0/794	1.53	5/1060 (0.5%)
9	U	1.26	0/797	1.44	7/1062 (0.7%)
10	Y	1.27	0/510	1.61	6/677 (0.9%)
11	1	0.91	0/1511	1.11	0/2354
12	2	0.91	0/867	1.17	3/1351 (0.2%)
13	3	2.00	16/1062 (1.5%)	1.76	21/1655 (1.3%)
14	4	2.01	46/2599 (1.8%)	1.88	93/4049 (2.3%)
All	All	1.84	333/18589 (1.8%)	2.04	915/27082 (3.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	y	2	18
2	E	0	2
3	G	0	1
4	n	3	0
5	p	0	29
6	a	0	1
7	5	0	3
9	U	0	1
11	1	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
12	2	0	2
13	3	0	19
14	4	0	63
All	All	5	141

All (333) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	n	99	ALA	C-N	40.18	1.89	1.33
4	n	22	TYR	C-N	38.43	1.84	1.33
13	3	1516	G	O3'-P	20.45	1.91	1.61
13	3	1551	A	O3'-P	14.37	1.82	1.61
1	y	350	GLY	CA-C	-10.51	1.42	1.52
3	G	19	LEU	N-CA	-10.09	1.34	1.46
7	5	60	ARG	CD-NE	10.02	1.60	1.46
7	5	220	ALA	N-CA	-9.83	1.39	1.46
1	y	336	VAL	CA-C	-9.69	1.41	1.52
2	E	96	ILE	N-CA	9.47	1.57	1.46
7	5	218	MET	C-N	9.40	1.43	1.33
7	5	171	ILE	CA-C	-9.23	1.42	1.52
7	5	74	ARG	CD-NE	8.86	1.58	1.46
3	G	48	SER	C-N	8.53	1.41	1.32
7	5	110	ASN	CA-CB	8.43	1.65	1.53
1	y	181	ARG	NE-CZ	8.36	1.42	1.33
1	y	200	PRO	CA-C	-8.29	1.44	1.52
5	p	52	A	C1'-N9	8.28	1.60	1.48
1	y	145	MET	CA-C	-8.23	1.42	1.52
1	y	74	ARG	CD-NE	8.14	1.57	1.46
5	p	58	A	C2'-C1'	-8.11	1.40	1.53
7	5	30	LEU	C-N	8.10	1.44	1.33
7	5	111	PHE	CA-C	-8.05	1.43	1.52
7	5	37	LYS	C-N	7.93	1.43	1.33
7	5	75	VAL	CA-C	-7.90	1.42	1.52
1	y	372	ARG	NE-CZ	7.88	1.41	1.33
1	y	380	TYR	CA-CB	7.78	1.65	1.53
1	y	278	ILE	CA-C	-7.76	1.43	1.52
7	5	175	ILE	C-N	7.74	1.40	1.33
7	5	145	VAL	N-CA	-7.73	1.39	1.46
1	y	180	GLU	C-N	7.67	1.43	1.33
7	5	76	ALA	C-N	7.63	1.43	1.33
1	y	71	ALA	CA-C	-7.60	1.43	1.52
3	G	70	LEU	N-CA	-7.58	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	4	2112	G	O5'-C5'	7.54	1.53	1.42
7	5	61	GLY	C-N	7.53	1.43	1.33
1	y	84	PRO	C-N	7.48	1.43	1.33
1	y	242	ARG	CD-NE	7.46	1.56	1.46
4	n	7	ALA	CA-C	-7.42	1.43	1.52
14	4	2199	A	C1'-N9	7.35	1.58	1.48
1	y	374	THR	N-CA	-7.29	1.37	1.46
1	y	205	HIS	CE1-NE2	7.27	1.39	1.32
14	4	2189	U	O4'-C1'	7.27	1.52	1.41
1	y	392	ARG	CA-CB	7.25	1.64	1.53
7	5	9	ARG	NE-CZ	7.25	1.41	1.33
3	G	51	PHE	C-N	7.18	1.43	1.33
14	4	2143	C	C5'-C4'	7.18	1.62	1.51
14	4	2150	C	O5'-C5'	7.17	1.53	1.42
1	y	88	ALA	C-N	7.16	1.43	1.33
1	y	327	PHE	CA-CB	7.08	1.64	1.53
1	y	51	LYS	C-N	7.05	1.42	1.33
7	5	2	ALA	CA-CB	7.03	1.65	1.53
1	y	176	GLU	C-N	6.99	1.42	1.33
1	y	194	GLY	C-N	6.98	1.42	1.33
1	y	54	GLU	CA-CB	6.98	1.64	1.53
7	5	12	ARG	CA-CB	6.92	1.64	1.53
1	y	219	VAL	CA-C	6.88	1.61	1.52
4	n	35	THR	CA-C	-6.88	1.43	1.52
5	p	20	U	C1'-N1	6.87	1.58	1.48
7	5	137	MET	C-N	6.87	1.42	1.33
1	y	41	ILE	CA-CB	6.85	1.63	1.54
14	4	2104	C	C1'-N1	6.84	1.58	1.48
1	y	237	VAL	CA-C	-6.83	1.44	1.52
13	3	1543	G	C2'-C1'	-6.82	1.43	1.53
1	y	275	ILE	CA-C	6.79	1.59	1.52
1	y	148	LEU	C-N	6.78	1.42	1.33
1	y	268	LYS	CA-CB	6.76	1.64	1.53
1	y	385	CYS	C-O	-6.74	1.16	1.24
14	4	2112	G	C5'-C4'	6.73	1.61	1.51
1	y	337	PHE	CA-CB	6.72	1.64	1.54
1	y	31	ILE	CA-C	-6.71	1.44	1.52
7	5	195	ALA	C-N	6.71	1.42	1.33
7	5	232	SER	CA-C	-6.70	1.44	1.52
2	E	79	VAL	CA-CB	-6.68	1.46	1.54
5	p	2	C	C1'-N1	6.66	1.58	1.48
14	4	2187	U	P-O5'	6.61	1.69	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	5	43	ASP	CA-C	-6.61	1.44	1.52
7	5	162	ARG	CZ-NH1	6.58	1.42	1.32
1	y	165	VAL	CA-C	-6.57	1.44	1.52
14	4	2166	U	O5'-C5'	6.56	1.52	1.42
1	y	16	LEU	C-N	6.56	1.42	1.33
1	y	266	PRO	C-N	6.55	1.43	1.33
1	y	340	ARG	CD-NE	6.55	1.55	1.46
1	y	416	PHE	CA-C	-6.55	1.44	1.52
5	p	24	G	C4'-C3'	6.55	1.62	1.52
1	y	227	VAL	CA-C	-6.54	1.44	1.52
1	y	322	ALA	CA-C	-6.53	1.44	1.52
7	5	131	LEU	N-CA	-6.50	1.38	1.45
1	y	311	GLN	CA-CB	6.48	1.62	1.53
7	5	28	ALA	C-N	6.47	1.42	1.33
7	5	186	LYS	C-N	6.46	1.42	1.33
14	4	2155	U	C5'-C4'	6.45	1.60	1.51
7	5	84	ALA	N-CA	-6.45	1.36	1.45
7	5	170	ILE	CA-C	-6.45	1.44	1.52
7	5	38	PHE	CA-CB	6.43	1.64	1.53
5	p	53	G	O5'-C5'	6.41	1.52	1.42
7	5	60	ARG	C-N	6.39	1.40	1.32
7	5	146	THR	CA-C	6.38	1.59	1.53
2	E	120	SER	C-N	6.36	1.42	1.33
3	G	46	SER	C-N	6.33	1.42	1.32
1	y	178	ILE	CA-C	-6.30	1.44	1.52
3	G	59	LEU	C-N	6.30	1.41	1.33
1	y	197	ALA	C-O	-6.28	1.16	1.24
2	E	92	HIS	CG-ND1	6.22	1.45	1.38
3	G	33	SER	CA-C	-6.22	1.44	1.52
14	4	2111	U	C1'-N1	6.18	1.57	1.48
2	E	113	GLY	N-CA	6.18	1.53	1.45
2	E	94	THR	N-CA	6.17	1.53	1.46
5	p	7	A	C1'-N9	6.17	1.56	1.47
1	y	60	ILE	CA-C	-6.16	1.45	1.52
2	E	126	ARG	CD-NE	6.15	1.54	1.46
3	G	53	THR	N-CA	-6.14	1.39	1.46
1	y	108	GLU	CA-CB	6.14	1.62	1.53
7	5	41	SER	CA-CB	6.13	1.61	1.53
1	y	118	GLN	CA-CB	6.13	1.62	1.53
1	y	86	ILE	CA-CB	-6.13	1.47	1.54
1	y	261	GLN	CA-CB	6.13	1.61	1.53
1	y	415	ASP	N-CA	-6.12	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	4	2189	U	C3'-C2'	-6.12	1.43	1.52
1	y	341	GLU	CA-CB	6.12	1.62	1.53
1	y	257	VAL	C-N	6.11	1.42	1.33
7	5	120	ALA	N-CA	-6.11	1.38	1.46
5	p	57	G	O3'-P	-6.10	1.52	1.61
5	p	2	C	C5'-C4'	6.10	1.60	1.51
2	E	83	ILE	N-CA	6.09	1.53	1.46
14	4	2114	A	C4'-C3'	6.09	1.61	1.52
7	5	74	ARG	NE-CZ	6.08	1.39	1.33
1	y	390	PHE	CA-C	-6.08	1.45	1.52
14	4	2104	C	P-O5'	-6.07	1.50	1.59
7	5	59	VAL	CA-CB	-6.06	1.46	1.54
1	y	70	GLY	CA-C	-6.06	1.43	1.51
1	y	300	TRP	C-N	6.05	1.41	1.33
3	G	33	SER	C-O	-6.04	1.17	1.24
14	4	2138	G	O5'-C5'	6.03	1.51	1.42
7	5	134	ARG	NE-CZ	6.03	1.39	1.33
7	5	119	ASP	C-N	6.01	1.42	1.33
1	y	422	THR	CA-C	-6.00	1.45	1.52
2	E	114	ILE	CB-CG1	5.99	1.65	1.53
7	5	86	ALA	CA-C	-5.98	1.44	1.52
3	G	57	ALA	CA-C	-5.98	1.45	1.52
1	y	153	GLY	C-N	5.98	1.41	1.33
3	G	60	ALA	N-CA	-5.98	1.39	1.46
14	4	2113	U	C5'-C4'	5.97	1.60	1.51
1	y	427	SER	N-CA	-5.96	1.39	1.46
5	p	30	C	P-O5'	-5.95	1.50	1.59
5	p	71	G	O3'-P	-5.94	1.52	1.61
5	p	70	C	C5'-C4'	5.93	1.60	1.51
3	G	68	LEU	C-N	5.92	1.41	1.33
1	y	244	ILE	CB-CG1	5.92	1.65	1.53
5	p	9	A	C4'-C3'	5.91	1.62	1.53
3	G	49	GLY	CA-C	-5.91	1.46	1.52
1	y	244	ILE	CA-CB	-5.91	1.46	1.53
3	G	40	ALA	CA-C	-5.90	1.45	1.52
7	5	164	ARG	NE-CZ	5.89	1.39	1.33
1	y	205	HIS	C-N	5.88	1.41	1.33
2	E	83	ILE	CA-C	-5.88	1.45	1.52
13	3	1521	G	O4'-C1'	5.87	1.50	1.41
1	y	257	VAL	CA-C	-5.85	1.45	1.52
13	3	1530	G	C5'-C4'	5.85	1.60	1.51
1	y	123	GLY	CA-C	-5.84	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	5	164	ARG	N-CA	-5.82	1.38	1.45
13	3	1543	G	C5'-C4'	5.82	1.59	1.51
14	4	2098	U	C1'-N1	5.82	1.57	1.48
7	5	48	LEU	N-CA	-5.81	1.38	1.45
14	4	2198	A	C1'-N9	-5.80	1.38	1.47
2	E	105	SER	CA-C	5.79	1.60	1.52
14	4	2093	G	C2'-C1'	-5.79	1.44	1.53
5	p	62	U	C5'-C4'	5.76	1.59	1.51
7	5	47	ASN	N-CA	-5.76	1.39	1.46
7	5	53	ARG	NE-CZ	5.76	1.39	1.33
7	5	139	ASN	N-CA	-5.76	1.42	1.46
2	E	87	ARG	NE-CZ	5.75	1.39	1.33
1	y	198	GLY	CA-C	-5.75	1.45	1.52
14	4	2156	G	O3'-P	-5.73	1.52	1.61
1	y	250	LYS	N-CA	-5.73	1.38	1.46
2	E	107	ILE	C-N	5.72	1.41	1.33
3	G	24	GLN	C-O	-5.72	1.17	1.24
3	G	42	LEU	CB-CG	5.70	1.64	1.53
1	y	37	SER	CA-CB	5.70	1.62	1.53
1	y	135	ILE	C-N	5.68	1.41	1.33
1	y	126	VAL	CA-CB	-5.67	1.47	1.54
3	G	18	GLY	C-N	5.66	1.41	1.33
1	y	336	VAL	CA-CB	5.66	1.64	1.54
7	5	88	LYS	N-CA	5.66	1.53	1.46
7	5	219	GLY	C-N	5.65	1.37	1.33
1	y	375	LEU	N-CA	5.64	1.53	1.46
14	4	2172	U	C4'-C3'	5.64	1.61	1.53
1	y	419	GLN	CA-C	-5.63	1.45	1.52
14	4	2130	U	C1'-N1	5.63	1.56	1.48
2	E	79	VAL	N-CA	-5.63	1.40	1.46
1	y	43	GLY	CA-C	-5.62	1.44	1.51
7	5	138	PRO	C-N	5.62	1.40	1.32
1	y	386	LEU	CA-C	-5.62	1.45	1.52
1	y	386	LEU	CA-CB	5.60	1.62	1.53
14	4	2172	U	C2'-C1'	-5.58	1.44	1.53
1	y	265	LEU	N-CA	-5.57	1.40	1.46
4	n	65	TYR	CA-CB	5.57	1.62	1.53
1	y	242	ARG	CZ-NH1	5.56	1.40	1.32
14	4	2152	G	O4'-C1'	5.56	1.50	1.41
14	4	2191	A	C5'-C4'	5.56	1.59	1.51
3	G	22	LEU	CA-C	-5.56	1.45	1.52
1	y	65	ASN	CA-C	5.55	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	4	2143	C	C4'-C3'	-5.54	1.44	1.52
1	y	283	ILE	CA-C	5.53	1.59	1.52
1	y	332	TYR	CA-CB	5.53	1.61	1.53
5	p	3	G	C4'-C3'	5.53	1.60	1.52
7	5	71	ARG	CZ-NH2	5.52	1.40	1.33
7	5	60	ARG	NE-CZ	5.52	1.39	1.33
4	n	4	ILE	N-CA	-5.52	1.40	1.46
1	y	304	THR	C-N	5.50	1.41	1.33
1	y	8	ASP	N-CA	-5.50	1.39	1.46
1	y	430	GLU	C-N	5.50	1.40	1.33
3	G	65	ILE	C-N	5.50	1.40	1.33
5	p	58	A	C3'-O3'	5.50	1.51	1.43
14	4	2171	A	C4'-C3'	5.49	1.61	1.53
1	y	357	ARG	CZ-NH2	5.49	1.40	1.33
1	y	229	ALA	CA-C	-5.48	1.45	1.52
4	n	69	GLN	N-CA	-5.48	1.39	1.45
14	4	2110	G	O3'-P	-5.47	1.52	1.61
1	y	245	VAL	CA-CB	-5.47	1.46	1.53
1	y	377	GLY	CA-C	-5.46	1.46	1.52
5	p	75	C	C1'-N1	5.45	1.56	1.48
7	5	98	GLU	N-CA	-5.45	1.42	1.47
1	y	125	LEU	C-N	5.45	1.40	1.33
1	y	224	ALA	CA-C	-5.44	1.46	1.52
1	y	79	ALA	N-CA	-5.43	1.39	1.46
14	4	2139	U	P-O5'	-5.43	1.51	1.59
7	5	51	ASP	CA-C	-5.42	1.45	1.52
7	5	183	ASP	CA-C	5.42	1.59	1.52
1	y	78	PHE	C-N	5.42	1.41	1.33
1	y	274	VAL	CA-CB	-5.42	1.48	1.54
2	E	87	ARG	CD-NE	5.41	1.53	1.46
13	3	1526	C	O5'-C5'	5.41	1.50	1.42
1	y	215	LEU	CA-C	-5.40	1.46	1.52
3	G	26	LYS	C-N	5.40	1.40	1.33
7	5	172	HIS	ND1-CE1	5.40	1.38	1.32
14	4	2141	G	C2-N3	5.40	1.43	1.32
1	y	246	VAL	CA-CB	-5.39	1.47	1.53
1	y	67	PHE	C-N	5.39	1.40	1.33
7	5	172	HIS	N-CA	5.38	1.53	1.46
1	y	415	ASP	C-N	5.38	1.40	1.33
1	y	191	ILE	CA-CB	-5.37	1.48	1.54
5	p	51	G	C4'-C3'	5.36	1.60	1.52
1	y	239	ARG	NE-CZ	5.36	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	38	ALA	CA-C	-5.35	1.45	1.52
1	y	407	LEU	N-CA	-5.35	1.39	1.46
7	5	33	LEU	C-N	5.35	1.40	1.33
14	4	2139	U	C5'-C4'	5.35	1.59	1.51
1	y	113	ARG	C-N	5.34	1.40	1.33
1	y	176	GLU	N-CA	5.33	1.52	1.46
1	y	379	LEU	C-N	5.33	1.40	1.33
2	E	109	TRP	N-CA	-5.32	1.40	1.46
14	4	2134	A	C2'-C1'	-5.31	1.45	1.53
2	E	86	THR	CB-OG1	-5.30	1.35	1.43
13	3	1526	C	C2'-O2'	-5.30	1.34	1.42
13	3	1543	G	C3'-C2'	5.29	1.60	1.52
4	n	85	PHE	C-N	5.29	1.41	1.33
5	p	58	A	O3'-P	-5.29	1.53	1.61
2	E	102	ALA	CA-CB	5.28	1.61	1.53
1	y	221	LEU	CA-C	5.28	1.59	1.52
7	5	121	MET	N-CA	-5.28	1.41	1.46
1	y	166	THR	CA-CB	5.28	1.61	1.53
1	y	394	ALA	CA-C	5.27	1.59	1.52
1	y	229	ALA	N-CA	-5.26	1.40	1.46
14	4	2107	G	C1'-N9	5.26	1.55	1.48
13	3	1524	G	C5'-C4'	5.25	1.59	1.51
7	5	21	TYR	C-N	5.25	1.40	1.33
5	p	68	C	O3'-P	-5.24	1.53	1.61
1	y	303	LEU	C-N	5.24	1.40	1.33
1	y	255	ARG	CZ-NH2	5.23	1.40	1.33
1	y	12	ALA	CA-C	-5.22	1.46	1.52
5	p	11	C	O4'-C1'	5.22	1.49	1.41
1	y	328	PHE	C-N	5.21	1.40	1.33
14	4	2113	U	C4'-C3'	5.21	1.60	1.52
7	5	58	ASN	CA-CB	5.20	1.61	1.53
5	p	56	C	C5'-C4'	5.20	1.59	1.51
1	y	157	TYR	N-CA	5.20	1.52	1.46
7	5	30	LEU	CA-C	-5.20	1.46	1.52
7	5	152	ALA	C-N	5.20	1.40	1.33
1	y	384	ILE	C-N	5.19	1.40	1.33
1	y	274	VAL	N-CA	-5.19	1.40	1.46
14	4	2126	A	C6-N6	5.19	1.44	1.33
1	y	292	SER	CA-C	-5.19	1.46	1.52
7	5	101	ALA	CA-C	-5.19	1.46	1.52
1	y	218	LEU	C-N	5.18	1.40	1.33
1	y	416	PHE	N-CA	5.18	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	4	2092	U	O3'-P	-5.18	1.53	1.61
1	y	372	ARG	CA-C	-5.17	1.46	1.52
2	E	89	GLU	C-O	-5.17	1.17	1.23
5	p	60	U	O3'-P	-5.17	1.53	1.61
1	y	36	GLY	CA-C	-5.16	1.45	1.52
7	5	154	LYS	CA-CB	5.16	1.61	1.53
5	p	20	U	C4'-O4'	5.15	1.53	1.45
7	5	220	ALA	C-N	5.15	1.39	1.33
14	4	2097	A	C5'-C4'	5.14	1.58	1.51
1	y	7	LEU	N-CA	-5.13	1.40	1.46
13	3	1518	C	C4'-O4'	-5.13	1.37	1.45
7	5	29	LEU	CA-C	-5.13	1.46	1.52
13	3	1529	G	C3'-O3'	-5.12	1.34	1.42
1	y	52	LEU	CA-C	-5.12	1.46	1.52
13	3	1518	C	P-O5'	-5.12	1.52	1.59
13	3	1539	U	C4'-C3'	-5.12	1.44	1.52
14	4	2182	U	C2'-C1'	-5.11	1.45	1.53
1	y	60	ILE	CB-CG1	5.10	1.63	1.53
14	4	2114	A	P-O5'	-5.10	1.52	1.59
14	4	2098	U	C2-N3	5.10	1.48	1.37
1	y	150	ILE	CB-CG1	5.09	1.63	1.53
13	3	1532	A	C5'-C4'	5.09	1.58	1.51
1	y	131	GLN	CA-C	-5.08	1.46	1.52
1	y	240	GLY	N-CA	-5.08	1.38	1.45
14	4	2100	G	C4'-O4'	5.08	1.53	1.45
1	y	149	VAL	N-CA	-5.07	1.40	1.46
1	y	283	ILE	C-N	5.07	1.40	1.33
1	y	249	ALA	CA-CB	-5.07	1.45	1.53
7	5	223	ALA	N-CA	-5.07	1.39	1.45
3	G	42	LEU	N-CA	-5.07	1.38	1.46
1	y	20	LYS	N-CA	-5.07	1.40	1.46
1	y	437	ASN	C-N	5.07	1.40	1.33
7	5	36	ALA	CA-C	-5.07	1.46	1.52
14	4	2135	A	P-O5'	5.06	1.67	1.59
3	G	54	ARG	NE-CZ	5.06	1.38	1.33
13	3	1521	G	C2'-C1'	-5.06	1.45	1.53
14	4	2120	G	O3'-P	-5.06	1.53	1.61
1	y	208	GLU	C-O	-5.05	1.18	1.24
1	y	235	VAL	CA-CB	-5.05	1.48	1.54
14	4	2148	G	N1-C2	5.05	1.47	1.37
14	4	2135	A	C5'-C4'	5.05	1.58	1.51
1	y	323	SER	N-CA	-5.05	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	y	217	PHE	CA-C	-5.03	1.46	1.52
1	y	128	ALA	CA-C	-5.03	1.46	1.52
14	4	2156	G	C2'-C1'	-5.03	1.45	1.53
1	y	400	TYR	CZ-OH	5.01	1.48	1.38
1	y	23	LEU	C-N	5.00	1.40	1.33

All (915) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	y	403	GLY	N-CA-C	30.48	152.45	114.66
1	y	56	GLN	N-CA-CB	20.17	144.58	110.49
4	n	41	ARG	N-CA-CB	17.51	140.09	110.49
4	n	46	ASP	N-CA-CB	17.15	139.47	110.49
1	y	404	THR	N-CA-CB	-15.60	87.06	110.61
4	n	41	ARG	CB-CA-C	-15.25	80.06	110.42
13	3	1551	A	P-O3'-C3'	14.14	141.42	120.20
4	n	40	GLN	N-CA-CB	14.08	134.28	110.49
4	n	40	GLN	CB-CA-C	13.94	138.16	110.42
2	E	92	HIS	CA-C-N	13.86	140.62	120.38
2	E	92	HIS	C-N-CA	13.86	140.62	120.38
4	n	71	LEU	N-CA-C	12.98	138.45	110.80
13	3	1516	G	O3'-P-O5'	12.38	122.57	104.00
2	E	96	ILE	CB-CA-C	-12.35	96.16	111.97
2	E	113	GLY	N-CA-C	12.29	126.75	112.50
1	y	55	GLN	N-CA-C	11.91	136.16	110.80
1	y	274	VAL	N-CA-C	11.84	121.78	110.42
4	n	41	ARG	N-CA-C	11.72	135.77	110.80
1	y	154	PHE	CA-CB-CG	-11.29	102.51	113.80
13	3	1551	A	OP2-P-O3'	-11.12	74.65	108.00
7	5	111	PHE	CA-CB-CG	-10.99	102.81	113.80
4	n	40	GLN	N-CA-C	-10.92	87.54	110.80
1	y	413	ILE	N-CA-C	10.79	120.78	110.42
13	3	1551	A	O3'-P-O5'	10.60	119.90	104.00
1	y	410	VAL	N-CA-C	10.48	120.48	110.42
2	E	83	ILE	CB-CA-C	-10.47	98.57	111.97
4	n	42	SER	N-CA-CB	10.40	128.07	110.49
1	y	391	MET	CA-C-N	10.33	134.12	120.28
1	y	391	MET	C-N-CA	10.33	134.12	120.28
4	n	39	HIS	N-CA-CB	10.26	127.82	110.49
2	E	93	THR	CA-C-N	10.15	134.28	120.38
2	E	93	THR	C-N-CA	10.15	134.28	120.38
3	G	51	PHE	CA-C-N	9.99	134.06	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	51	PHE	C-N-CA	9.99	134.06	120.38
2	E	86	THR	N-CA-CB	9.98	124.48	110.01
3	G	34	PHE	CA-CB-CG	9.90	123.70	113.80
1	y	173	TRP	CA-C-N	9.83	133.22	120.44
1	y	173	TRP	C-N-CA	9.83	133.22	120.44
14	4	2175	C	P-O3'-C3'	9.73	134.79	120.20
7	5	27	ILE	CA-C-O	-9.71	110.56	120.85
1	y	423	LEU	N-CA-C	9.64	121.39	111.07
1	y	414	MET	CA-C-N	9.52	132.82	120.44
1	y	414	MET	C-N-CA	9.52	132.82	120.44
14	4	2153	C	P-O5'-C5'	-9.52	106.61	120.90
2	E	117	ARG	N-CA-C	9.45	121.18	111.07
1	y	393	ASP	CA-C-O	-9.39	110.96	120.82
1	y	295	GLY	CA-C-N	9.37	130.34	119.94
1	y	295	GLY	C-N-CA	9.37	130.34	119.94
1	y	240	GLY	CA-C-N	9.37	136.21	123.00
1	y	240	GLY	C-N-CA	9.37	136.21	123.00
3	G	36	ALA	CB-CA-C	-9.29	96.61	111.28
5	p	12	U	P-O5'-C5'	9.27	134.81	120.90
1	y	61	ILE	CA-C-O	-9.26	111.36	121.17
1	y	65	ASN	CA-CB-CG	9.22	121.82	112.60
2	E	114	ILE	CB-CA-C	9.22	124.59	112.14
1	y	335	LEU	O-C-N	9.21	131.56	122.07
1	y	57	ARG	NE-CZ-NH2	9.19	127.47	119.20
1	y	340	ARG	CA-C-N	9.17	132.36	120.44
1	y	340	ARG	C-N-CA	9.17	132.36	120.44
1	y	308	LEU	CA-C-N	9.16	132.56	120.28
1	y	308	LEU	C-N-CA	9.16	132.56	120.28
1	y	416	PHE	CA-CB-CG	9.13	122.93	113.80
1	y	101	THR	CA-C-N	9.13	132.52	120.28
1	y	101	THR	C-N-CA	9.13	132.52	120.28
1	y	315	PRO	CA-C-N	9.10	138.92	121.54
1	y	315	PRO	C-N-CA	9.10	138.92	121.54
1	y	39	ILE	CA-C-N	9.07	131.18	119.84
1	y	39	ILE	C-N-CA	9.07	131.18	119.84
1	y	45	ASP	CA-CB-CG	9.07	121.67	112.60
1	y	311	GLN	CA-C-O	-9.04	110.01	118.33
1	y	85	TYR	CA-C-N	9.04	131.95	120.56
1	y	85	TYR	C-N-CA	9.04	131.95	120.56
1	y	415	ASP	N-CA-C	8.95	120.64	111.07
13	3	1537	G	P-O3'-C3'	8.95	133.62	120.20
14	4	2161	C	P-O3'-C3'	8.93	133.59	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	n	38	LEU	N-CA-C	8.84	129.62	110.80
3	G	67	SER	N-CA-C	8.75	120.43	111.07
1	y	424	MET	N-CA-CB	8.70	122.62	110.01
12	2	1315	C	P-O3'-C3'	8.63	133.14	120.20
1	y	337	PHE	N-CA-C	-8.56	101.98	114.39
1	y	319	LEU	N-CA-C	8.56	120.22	111.07
7	5	179	ASP	N-CA-C	-8.50	103.03	112.72
1	y	288	ALA	CA-C-N	8.44	131.59	120.28
1	y	288	ALA	C-N-CA	8.44	131.59	120.28
1	y	81	GLY	CA-C-N	8.37	131.93	120.46
1	y	81	GLY	C-N-CA	8.37	131.93	120.46
1	y	352	PHE	CA-CB-CG	8.38	122.17	113.80
1	y	67	PHE	CA-C-N	8.37	131.84	120.54
1	y	67	PHE	C-N-CA	8.37	131.84	120.54
4	n	99	ALA	CA-C-N	-8.35	106.67	121.70
4	n	99	ALA	C-N-CA	-8.35	106.67	121.70
1	y	46	ALA	N-CA-C	8.34	120.00	111.07
7	5	22	ASP	CA-CB-CG	-8.29	104.31	112.60
1	y	294	PHE	CA-C-N	8.28	129.13	119.94
1	y	294	PHE	C-N-CA	8.28	129.13	119.94
4	n	2	LYS	CA-C-N	8.28	131.38	120.28
4	n	2	LYS	C-N-CA	8.28	131.38	120.28
1	y	139	LEU	CA-C-N	8.26	127.56	118.97
1	y	139	LEU	C-N-CA	8.26	127.56	118.97
1	y	166	THR	N-CA-CB	8.16	122.11	110.12
1	y	238	GLU	N-CA-CB	8.14	122.06	109.94
1	y	283	ILE	N-CA-C	8.12	118.90	110.62
3	G	34	PHE	N-CA-CB	8.11	124.20	110.49
1	y	172	MET	CA-C-N	8.09	130.96	120.44
1	y	172	MET	C-N-CA	8.09	130.96	120.44
1	y	340	ARG	NE-CZ-NH2	8.08	126.47	119.20
3	G	49	GLY	CA-C-O	-8.01	116.52	122.37
1	y	89	SER	CA-C-N	8.01	130.65	120.56
1	y	89	SER	C-N-CA	8.01	130.65	120.56
14	4	2105	U	O4'-C4'-C3'	-7.98	96.02	104.00
2	E	84	TRP	CA-C-N	7.92	127.84	119.05
2	E	84	TRP	C-N-CA	7.92	127.84	119.05
1	y	205	HIS	ND1-CE1-NE2	7.88	116.28	108.40
3	G	33	SER	CA-C-N	7.88	136.59	121.54
3	G	33	SER	C-N-CA	7.88	136.59	121.54
7	5	42	VAL	N-CA-CB	7.88	119.31	110.72
1	y	255	ARG	N-CA-CB	7.88	123.80	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	p	63	C	O4'-C1'-N1	7.86	120.29	108.50
1	y	105	ILE	CA-C-N	7.86	130.65	120.44
1	y	105	ILE	C-N-CA	7.86	130.65	120.44
2	E	80	ARG	CA-C-N	7.84	131.13	120.54
2	E	80	ARG	C-N-CA	7.84	131.13	120.54
7	5	94	LEU	CA-C-N	-7.83	114.29	121.65
7	5	94	LEU	C-N-CA	-7.83	114.29	121.65
1	y	350	GLY	O-C-N	7.75	130.60	122.93
3	G	22	LEU	CA-C-N	7.74	130.50	120.44
3	G	22	LEU	C-N-CA	7.74	130.50	120.44
1	y	202	ALA	N-CA-C	7.73	120.39	111.11
7	5	194	VAL	CA-C-N	7.71	130.47	120.44
7	5	194	VAL	C-N-CA	7.71	130.47	120.44
7	5	28	ALA	CA-C-N	7.71	130.46	120.44
7	5	28	ALA	C-N-CA	7.71	130.46	120.44
1	y	376	VAL	CA-C-N	7.69	128.52	119.98
1	y	376	VAL	C-N-CA	7.69	128.52	119.98
1	y	178	ILE	N-CA-C	7.69	118.46	110.62
7	5	67	HIS	CA-C-N	7.68	131.91	121.01
7	5	67	HIS	C-N-CA	7.68	131.91	121.01
7	5	26	ALA	CA-C-N	7.67	131.32	120.42
7	5	26	ALA	C-N-CA	7.67	131.32	120.42
14	4	2145	C	P-O5'-C5'	7.66	132.40	120.90
1	y	16	LEU	CA-C-N	7.66	128.65	119.99
1	y	16	LEU	C-N-CA	7.66	128.65	119.99
1	y	353	VAL	CA-C-O	-7.66	112.47	119.82
1	y	237	VAL	N-CA-C	7.66	117.77	110.42
3	G	58	LEU	O-C-N	7.64	130.22	122.12
1	y	298	THR	N-CA-CB	7.63	123.39	110.49
3	G	70	LEU	CA-C-N	7.63	128.45	119.98
3	G	70	LEU	C-N-CA	7.63	128.45	119.98
7	5	94	LEU	N-CA-CB	7.62	123.38	111.56
14	4	2142	A	P-O5'-C5'	-7.62	109.47	120.90
3	G	20	ILE	CA-C-N	7.62	130.34	120.44
3	G	20	ILE	C-N-CA	7.62	130.34	120.44
7	5	224	VAL	CA-C-N	7.60	132.36	121.50
7	5	224	VAL	C-N-CA	7.60	132.36	121.50
1	y	109	GLY	N-CA-C	7.59	121.31	112.50
1	y	228	PHE	N-CA-C	7.58	119.18	111.07
14	4	2138	G	C4'-C3'-C2'	-7.57	95.03	102.60
5	p	42	C	O4'-C4'-C3'	-7.57	96.44	104.00
1	y	8	ASP	CB-CA-C	7.55	123.52	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	41	THR	N-CA-C	-7.55	103.63	112.92
1	y	35	ILE	N-CA-CB	7.51	119.34	110.55
1	y	242	ARG	NE-CZ-NH2	7.50	125.95	119.20
1	y	266	PRO	CA-C-N	-7.50	111.81	123.13
1	y	266	PRO	C-N-CA	-7.50	111.81	123.13
2	E	105	SER	N-CA-CB	7.50	121.14	110.12
14	4	2093	G	C4'-C3'-C2'	-7.48	95.12	102.60
14	4	2100	G	P-O5'-C5'	-7.48	109.67	120.90
3	G	13	ALA	N-CA-C	7.47	119.42	111.28
1	y	141	ASN	N-CA-C	7.41	118.99	111.07
8	T	22	THR	N-CA-C	-7.40	104.10	113.43
1	y	37	SER	N-CA-C	7.39	118.98	111.07
2	E	88	GLN	CA-C-N	7.38	132.85	122.36
2	E	88	GLN	C-N-CA	7.38	132.85	122.36
1	y	335	LEU	CA-C-O	-7.38	113.07	120.82
2	E	89	GLU	N-CA-CB	7.35	122.58	111.70
7	5	101	ALA	CB-CA-C	-7.35	99.33	110.88
1	y	66	MET	N-CA-C	7.35	118.94	111.07
7	5	134	ARG	N-CA-C	-7.35	104.29	113.55
1	y	268	LYS	CA-C-O	-7.35	112.45	120.24
1	y	192	PHE	CA-C-N	7.33	130.10	120.28
1	y	192	PHE	C-N-CA	7.33	130.10	120.28
3	G	30	MET	CA-C-O	-7.32	113.13	120.82
5	p	17	U	C1'-O4'-C4'	-7.32	102.58	109.90
1	y	126	VAL	CA-C-N	7.31	129.94	120.44
1	y	126	VAL	C-N-CA	7.31	129.94	120.44
1	y	45	ASP	N-CA-CB	7.28	122.79	110.49
1	y	72	LEU	N-CA-C	-7.26	101.53	110.61
5	p	46	G	P-O3'-C3'	7.25	131.08	120.20
14	4	2171	A	P-O5'-C5'	7.24	131.76	120.90
1	y	22	ARG	CA-C-N	7.24	129.85	120.44
1	y	22	ARG	C-N-CA	7.24	129.85	120.44
13	3	1541	C	O4'-C1'-N1	7.23	119.34	108.50
1	y	61	ILE	N-CA-C	7.22	117.36	110.42
1	y	438	LEU	N-CA-CB	7.20	122.66	110.49
5	p	3	G	P-O3'-C3'	7.20	131.00	120.20
7	5	227	ALA	N-CA-C	-7.18	104.66	113.50
7	5	168	ASN	CA-CB-CG	-7.18	105.42	112.60
8	T	25	GLU	N-CA-C	-7.17	106.45	114.62
7	5	110	ASN	N-CA-C	-7.16	103.10	112.41
2	E	114	ILE	N-CA-CB	7.14	120.25	110.54
3	G	33	SER	CA-C-O	-7.13	112.99	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	y	414	MET	O-C-N	7.13	129.42	122.07
1	y	191	ILE	CA-C-N	7.10	129.80	120.28
1	y	191	ILE	C-N-CA	7.10	129.80	120.28
14	4	2172	U	C2'-C3'-O3'	7.10	120.15	109.50
1	y	205	HIS	ND1-CG-CD2	7.09	113.19	106.10
1	y	233	PHE	CA-C-N	7.09	129.49	120.56
1	y	233	PHE	C-N-CA	7.09	129.49	120.56
2	E	104	MET	CA-C-N	7.09	129.78	120.28
2	E	104	MET	C-N-CA	7.09	129.78	120.28
14	4	2180	U	C4'-C3'-C2'	-7.08	95.52	102.60
1	y	27	ILE	CA-C-N	7.07	127.79	119.94
1	y	27	ILE	C-N-CA	7.07	127.79	119.94
1	y	47	ALA	CB-CA-C	-7.06	99.79	110.88
8	T	88	LYS	N-CA-C	-7.04	105.62	114.56
1	y	286	PHE	CA-CB-CG	7.03	120.83	113.80
1	y	149	VAL	N-CA-C	-7.02	105.20	113.42
3	G	19	LEU	N-CA-C	7.02	118.93	111.28
1	y	190	ILE	CA-C-N	7.00	129.38	120.56
1	y	190	ILE	C-N-CA	7.00	129.38	120.56
1	y	432	ALA	CA-C-O	6.97	128.14	120.82
3	G	24	GLN	CA-C-N	6.97	127.87	119.99
3	G	24	GLN	C-N-CA	6.97	127.87	119.99
7	5	21	TYR	N-CA-C	-6.97	98.71	109.52
1	y	151	ASN	CA-C-N	6.93	128.50	119.84
1	y	151	ASN	C-N-CA	6.93	128.50	119.84
1	y	82	ILE	CA-C-O	-6.92	113.75	120.95
1	y	53	LEU	CA-C-O	-6.92	113.56	120.82
7	5	101	ALA	CA-C-N	6.90	129.85	120.54
7	5	101	ALA	C-N-CA	6.90	129.85	120.54
3	G	68	LEU	N-CA-C	6.86	118.76	111.28
7	5	124	VAL	N-CA-C	-6.85	97.87	107.80
1	y	307	SER	CA-C-N	6.84	129.45	120.28
1	y	307	SER	C-N-CA	6.84	129.45	120.28
7	5	231	ALA	N-CA-C	-6.84	104.92	112.72
13	3	1549	A	O5'-C5'-C4'	-6.84	101.24	111.50
12	2	1333	G	P-O3'-C3'	6.84	130.46	120.20
1	y	83	MET	CA-C-O	-6.82	112.05	118.73
3	G	28	ALA	CA-C-N	6.81	129.29	120.44
3	G	28	ALA	C-N-CA	6.81	129.29	120.44
2	E	127	PHE	CA-CB-CG	6.81	120.61	113.80
5	p	14	A	O5'-C5'-C4'	-6.80	101.30	111.50
1	y	420	VAL	N-CA-CB	6.80	118.06	110.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	y	267	LEU	CA-C-N	6.79	132.34	122.77
1	y	267	LEU	C-N-CA	6.79	132.34	122.77
1	y	140	PRO	CA-C-N	6.79	129.27	120.44
1	y	140	PRO	C-N-CA	6.79	129.27	120.44
14	4	2185	U	P-O5'-C5'	-6.79	110.72	120.90
1	y	184	GLY	CA-C-N	6.78	134.49	121.54
1	y	184	GLY	C-N-CA	6.78	134.49	121.54
1	y	186	GLY	CA-C-N	6.77	129.73	120.46
1	y	186	GLY	C-N-CA	6.77	129.73	120.46
5	p	64	G	O4'-C1'-N9	6.75	118.63	108.50
3	G	48	SER	N-CA-CB	6.74	120.73	109.94
14	4	2167	U	P-O5'-C5'	6.74	131.01	120.90
3	G	66	ILE	N-CA-CB	6.74	118.43	110.55
1	y	60	ILE	N-CA-C	6.73	116.88	110.42
1	y	394	ALA	CA-C-N	6.73	129.30	120.28
1	y	394	ALA	C-N-CA	6.73	129.30	120.28
2	E	108	LEU	CA-C-N	6.73	129.19	120.44
2	E	108	LEU	C-N-CA	6.73	129.19	120.44
1	y	224	ALA	CA-C-N	6.73	129.68	120.46
1	y	224	ALA	C-N-CA	6.73	129.68	120.46
1	y	47	ALA	N-CA-CB	6.72	119.76	110.01
5	p	17	U	O4'-C1'-C2'	6.71	114.31	107.60
1	y	264	HIS	CA-CB-CG	6.71	120.51	113.80
1	y	419	GLN	N-CA-C	6.70	118.24	111.07
14	4	2165	C	C3'-C2'-C1'	6.68	107.98	101.30
1	y	300	TRP	CB-CG-CD2	6.67	136.14	126.80
7	5	65	LEU	CA-C-N	6.67	127.53	120.12
7	5	65	LEU	C-N-CA	6.67	127.53	120.12
1	y	369	VAL	O-C-N	6.67	128.45	121.91
1	y	410	VAL	O-C-N	-6.67	115.37	121.91
7	5	23	ILE	CA-C-N	6.66	129.75	120.29
7	5	23	ILE	C-N-CA	6.66	129.75	120.29
7	5	209	ILE	N-CA-CB	6.66	119.50	111.31
1	y	421	GLN	CA-C-N	6.66	129.10	120.44
1	y	421	GLN	C-N-CA	6.66	129.10	120.44
7	5	42	VAL	N-CA-C	-6.66	98.99	108.58
3	G	71	GLY	CA-C-N	6.65	133.48	121.97
3	G	71	GLY	C-N-CA	6.65	133.48	121.97
3	G	30	MET	N-CA-C	6.63	118.17	111.07
5	p	1	G	C4'-C3'-C2'	-6.62	95.98	102.60
14	4	2167	U	O4'-C1'-N1	6.62	118.43	108.50
1	y	7	LEU	CA-C-N	6.62	129.45	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	y	7	LEU	C-N-CA	6.62	129.45	120.38
1	y	102	LEU	CA-C-N	6.62	129.04	120.44
1	y	102	LEU	C-N-CA	6.62	129.04	120.44
2	E	101	THR	CA-C-N	6.62	129.04	120.44
2	E	101	THR	C-N-CA	6.62	129.04	120.44
1	y	217	PHE	CA-CB-CG	6.62	120.42	113.80
7	5	72	SER	N-CA-CB	6.61	121.66	110.49
2	E	107	ILE	CA-C-N	6.60	129.02	120.44
2	E	107	ILE	C-N-CA	6.60	129.02	120.44
1	y	14	GLY	CA-C-N	6.59	127.25	119.94
1	y	14	GLY	C-N-CA	6.59	127.25	119.94
5	p	24	G	O4'-C1'-N9	6.59	118.39	108.50
7	5	46	VAL	CA-C-N	6.58	131.18	122.30
7	5	46	VAL	C-N-CA	6.58	131.18	122.30
1	y	14	GLY	CA-C-O	-6.58	113.98	120.75
7	5	159	GLY	CA-C-N	6.57	132.44	122.65
7	5	159	GLY	C-N-CA	6.57	132.44	122.65
7	5	27	ILE	CA-C-N	6.56	129.08	120.28
7	5	27	ILE	C-N-CA	6.56	129.08	120.28
1	y	243	ARG	CB-CA-C	6.55	121.29	110.74
1	y	127	LEU	CA-C-N	6.55	128.96	120.44
1	y	127	LEU	C-N-CA	6.55	128.96	120.44
1	y	366	ILE	CA-C-N	6.54	129.35	120.38
1	y	366	ILE	C-N-CA	6.54	129.35	120.38
14	4	2155	U	O5'-C5'-C4'	6.54	121.32	111.50
1	y	209	GLN	OE1-CD-NE2	-6.54	116.06	122.60
1	y	196	VAL	CA-C-N	6.54	129.04	120.28
1	y	196	VAL	C-N-CA	6.54	129.04	120.28
1	y	293	TRP	CA-C-N	6.54	128.94	120.44
1	y	293	TRP	C-N-CA	6.54	128.94	120.44
1	y	230	VAL	O-C-N	6.53	128.31	121.91
1	y	397	VAL	CB-CA-C	6.51	116.99	110.94
7	5	6	LYS	CA-C-N	6.50	129.65	120.28
7	5	6	LYS	C-N-CA	6.50	129.65	120.28
1	y	174	LEU	O-C-N	6.50	128.77	122.07
1	y	373	LEU	CA-C-O	6.50	127.64	120.82
1	y	119	TYR	CB-CG-CD1	6.49	130.54	120.80
1	y	330	PHE	CA-CB-CG	-6.49	107.31	113.80
1	y	123	GLY	CA-C-N	6.49	128.87	120.44
1	y	123	GLY	C-N-CA	6.49	128.87	120.44
1	y	268	LYS	CB-CG-CD	6.48	126.20	111.30
5	p	64	G	P-O3'-C3'	-6.47	110.50	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	y	8	ASP	CA-C-N	6.47	128.85	120.44
1	y	8	ASP	C-N-CA	6.47	128.85	120.44
1	y	139	LEU	N-CA-CB	6.46	119.92	110.30
1	y	205	HIS	CA-C-O	-6.46	114.04	120.82
14	4	2147	A	C4'-C3'-O3'	-6.46	103.31	113.00
2	E	88	GLN	N-CA-CB	6.45	121.39	110.49
1	y	11	SER	CA-C-N	6.44	128.82	120.44
1	y	11	SER	C-N-CA	6.44	128.82	120.44
1	y	93	GLN	CA-C-O	-6.44	113.72	120.55
2	E	118	LEU	CA-C-N	6.43	129.27	120.46
2	E	118	LEU	C-N-CA	6.43	129.27	120.46
1	y	347	LYS	CB-CA-C	-6.43	100.79	110.88
7	5	48	LEU	N-CA-C	-6.43	100.10	110.32
13	3	1525	A	C4'-C3'-O3'	-6.42	103.37	113.00
1	y	223	VAL	CB-CA-C	-6.41	103.48	112.14
13	3	1520	U	O4'-C1'-N1	6.41	118.11	108.50
1	y	256	ARG	CA-C-N	6.40	129.39	121.71
1	y	256	ARG	C-N-CA	6.40	129.39	121.71
7	5	188	ASN	OD1-CG-ND2	6.39	128.99	122.60
1	y	181	ARG	CB-CA-C	-6.38	100.86	110.88
3	G	11	ILE	CA-CB-CG2	-6.38	99.66	110.50
7	5	59	VAL	N-CA-C	-6.37	98.57	107.80
5	p	10	G	P-O5'-C5'	-6.36	111.36	120.90
4	n	3	LYS	CA-C-N	6.35	129.16	120.46
4	n	3	LYS	C-N-CA	6.35	129.16	120.46
3	G	73	ILE	N-CA-CB	6.34	122.28	111.50
7	5	108	GLU	N-CA-CB	6.34	121.12	110.79
13	3	1546	G	O5'-C5'-C4'	-6.33	102.00	111.50
2	E	112	ASP	O-C-N	-6.33	115.55	122.07
3	G	70	LEU	O-C-N	6.33	128.59	122.07
5	p	34	G	O4'-C1'-N9	6.33	117.99	108.50
1	y	195	ILE	CA-C-N	6.32	128.75	120.60
1	y	195	ILE	C-N-CA	6.32	128.75	120.60
14	4	2193	G	C5'-C4'-O4'	6.32	119.28	109.80
2	E	96	ILE	CA-CB-CG1	6.32	121.14	110.40
5	p	16	U	P-O3'-C3'	6.31	129.67	120.20
5	p	13	C	C5'-C4'-C3'	-6.31	106.53	116.00
7	5	30	LEU	CA-C-N	6.31	128.64	120.44
7	5	30	LEU	C-N-CA	6.31	128.64	120.44
1	y	25	PHE	N-CA-CB	6.31	119.39	110.12
1	y	341	GLU	CA-C-N	6.30	128.63	120.44
1	y	341	GLU	C-N-CA	6.30	128.63	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	T	2	ILE	N-CA-C	-6.29	106.67	112.96
3	G	41	THR	CA-CB-OG1	6.29	119.03	109.60
14	4	2189	U	O4'-C1'-N1	6.28	117.92	108.50
5	p	57	G	P-O3'-C3'	6.28	129.61	120.20
14	4	2178	C	O4'-C1'-N1	6.27	117.90	108.50
1	y	211	ARG	N-CA-C	-6.27	100.08	110.17
1	y	99	HIS	CB-CG-CD2	-6.26	123.06	131.20
14	4	2181	U	C5'-C4'-O4'	6.26	119.19	109.80
3	G	34	PHE	N-CA-C	-6.26	97.47	110.80
7	5	98	GLU	O-C-N	-6.26	116.03	121.85
3	G	18	GLY	CA-C-N	6.25	128.66	120.28
3	G	18	GLY	C-N-CA	6.25	128.66	120.28
8	T	95	PHE	CA-CB-CG	-6.25	107.55	113.80
14	4	2105	U	O4'-C1'-N1	6.24	117.86	108.50
3	G	23	GLN	N-CA-C	-6.24	104.40	111.07
1	y	187	ILE	N-CA-C	-6.23	104.26	110.62
14	4	2196	C	O4'-C1'-N1	6.23	117.84	108.50
1	y	173	TRP	N-CA-CB	6.23	119.04	110.01
1	y	279	PHE	N-CA-C	6.22	117.72	111.07
1	y	338	ASN	O-C-N	-6.21	114.65	120.55
2	E	79	VAL	N-CA-CB	-6.20	103.30	110.55
1	y	64	PHE	CA-CB-CG	-6.20	107.60	113.80
1	y	283	ILE	CA-C-N	6.20	128.37	120.56
1	y	283	ILE	C-N-CA	6.20	128.37	120.56
4	n	7	ALA	CA-C-N	6.19	128.49	120.44
4	n	7	ALA	C-N-CA	6.19	128.49	120.44
2	E	92	HIS	ND1-CE1-NE2	6.19	114.59	108.40
2	E	121	PHE	CA-CB-CG	6.19	119.99	113.80
1	y	41	ILE	CA-C-N	6.18	125.80	119.56
1	y	41	ILE	C-N-CA	6.18	125.80	119.56
1	y	39	ILE	CA-C-O	-6.17	113.97	119.71
1	y	168	THR	CA-CB-CG2	6.16	120.98	110.50
7	5	53	ARG	CA-C-N	6.16	131.15	122.46
7	5	53	ARG	C-N-CA	6.16	131.15	122.46
1	y	217	PHE	CA-C-O	-6.16	114.35	120.82
1	y	40	PRO	CA-N-CD	-6.15	103.39	112.00
1	y	383	PHE	CA-C-O	-6.15	114.03	120.55
7	5	103	GLN	OE1-CD-NE2	-6.15	116.45	122.60
1	y	372	ARG	N-CA-CB	6.14	118.92	110.01
14	4	2123	G	C4'-C3'-C2'	-6.14	96.46	102.60
2	E	122	ILE	O-C-N	-6.14	115.90	121.91
1	y	261	GLN	N-CA-C	-6.13	99.86	109.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	4	2180	U	C5'-C4'-C3'	-6.13	106.80	116.00
5	p	13	C	P-O3'-C3'	-6.13	111.00	120.20
1	y	215	LEU	CA-C-N	6.12	128.40	120.44
1	y	215	LEU	C-N-CA	6.12	128.40	120.44
1	y	17	GLY	O-C-N	6.12	128.19	122.13
1	y	99	HIS	ND1-CG-CD2	6.12	112.22	106.10
1	y	57	ARG	N-CA-C	6.12	123.84	110.80
1	y	91	ILE	CA-C-N	6.12	128.84	120.46
1	y	91	ILE	C-N-CA	6.12	128.84	120.46
1	y	439	LYS	N-CA-CB	6.12	120.83	110.49
1	y	290	ILE	CA-C-N	6.11	128.38	120.44
1	y	290	ILE	C-N-CA	6.11	128.38	120.44
5	p	61	C	P-O5'-C5'	6.09	130.03	120.90
1	y	340	ARG	N-CA-C	-6.09	97.27	107.80
5	p	39	G	P-O3'-C3'	-6.08	111.07	120.20
1	y	308	LEU	CA-C-O	-6.08	114.10	120.55
1	y	240	GLY	O-C-N	6.08	130.60	122.70
1	y	385	CYS	CA-C-N	6.08	128.43	120.28
1	y	385	CYS	C-N-CA	6.08	128.43	120.28
1	y	61	ILE	N-CA-CB	6.08	117.66	110.55
14	4	2173	A	C5'-C4'-C3'	6.08	125.12	116.00
1	y	384	ILE	O-C-N	6.08	127.86	121.91
6	a	9	A	C2'-C3'-O3'	6.07	122.80	113.70
3	G	31	GLY	N-CA-C	6.06	127.55	113.18
1	y	197	ALA	CA-C-N	6.05	126.70	119.98
1	y	197	ALA	C-N-CA	6.05	126.70	119.98
7	5	110	ASN	OD1-CG-ND2	6.05	128.65	122.60
14	4	2096	C	O5'-C5'-C4'	-6.04	102.43	111.50
1	y	165	VAL	CB-CA-C	-6.04	103.99	112.14
1	y	40	PRO	N-CA-C	6.04	124.91	112.47
4	n	87	THR	CA-CB-OG1	6.04	118.65	109.60
7	5	44	VAL	O-C-N	-6.03	116.85	123.18
1	y	77	ILE	N-CA-C	-6.03	99.19	107.75
1	y	40	PRO	N-CD-CG	6.02	112.24	103.20
1	y	118	GLN	CA-C-N	6.02	128.27	120.44
1	y	118	GLN	C-N-CA	6.02	128.27	120.44
7	5	26	ALA	N-CA-C	6.02	118.34	111.11
14	4	2146	C	C3'-C2'-C1'	6.02	107.32	101.30
1	y	269	VAL	O-C-N	-6.02	116.82	123.20
1	y	427	SER	CA-C-N	6.01	128.26	120.44
1	y	427	SER	C-N-CA	6.01	128.26	120.44
14	4	2133	G	C1'-O4'-C4'	-6.01	103.69	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	5	217	THR	O-C-N	6.01	129.75	122.96
1	y	384	ILE	N-CA-CB	6.00	117.58	110.55
2	E	125	LEU	N-CA-C	5.99	117.48	111.07
1	y	193	ALA	O-C-N	5.99	128.47	122.12
7	5	102	ASP	CA-C-O	-5.99	114.49	120.90
5	p	20	U	C5'-C4'-C3'	-5.98	107.02	116.00
1	y	177	GLN	CA-C-N	5.98	128.66	120.46
1	y	177	GLN	C-N-CA	5.98	128.66	120.46
1	y	185	ASN	CA-CB-CG	-5.98	106.62	112.60
5	p	48	C	O4'-C1'-C2'	-5.97	101.63	107.60
1	y	382	THR	CA-CB-OG1	5.97	118.55	109.60
1	y	394	ALA	CB-CA-C	-5.97	101.51	110.88
1	y	261	GLN	OE1-CD-NE2	5.96	128.56	122.60
13	3	1523	U	C3'-C2'-C1'	5.96	107.26	101.30
7	5	129	GLN	OE1-CD-NE2	-5.96	116.64	122.60
2	E	121	PHE	CA-C-N	5.95	128.06	120.56
2	E	121	PHE	C-N-CA	5.95	128.06	120.56
7	5	208	TYR	N-CA-CB	5.95	120.55	110.49
7	5	211	LYS	O-C-N	-5.94	115.47	122.96
3	G	50	ASN	N-CA-C	-5.94	99.72	109.40
13	3	1552	A	P-O5'-C5'	5.93	129.80	120.90
1	y	32	VAL	CB-CA-C	5.93	119.56	111.97
1	y	433	LEU	N-CA-C	5.93	117.41	111.07
1	y	85	TYR	CB-CA-C	-5.92	101.59	110.88
1	y	404	THR	N-CA-C	-5.91	105.38	113.30
1	y	440	GLY	CA-C-O	-5.91	108.39	120.80
1	y	118	GLN	CB-CA-C	-5.91	101.61	110.88
1	y	382	THR	CA-C-N	5.90	128.19	120.28
1	y	382	THR	C-N-CA	5.90	128.19	120.28
1	y	67	PHE	CA-CB-CG	5.90	119.70	113.80
1	y	158	PHE	CA-C-N	5.90	128.11	120.44
1	y	158	PHE	C-N-CA	5.90	128.11	120.44
5	p	69	C	P-O3'-C3'	5.90	129.05	120.20
14	4	2197	U	C2'-C3'-O3'	5.90	118.35	109.50
1	y	257	VAL	N-CA-C	-5.90	107.75	113.53
7	5	53	ARG	N-CA-C	-5.89	98.68	108.75
1	y	190	ILE	CB-CA-C	5.88	119.50	111.97
1	y	198	GLY	CA-C-N	5.87	127.43	120.09
1	y	198	GLY	C-N-CA	5.87	127.43	120.09
1	y	432	ALA	CA-C-N	5.87	128.07	120.44
1	y	432	ALA	C-N-CA	5.87	128.07	120.44
3	G	62	LEU	CA-C-N	5.87	128.15	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	62	LEU	C-N-CA	5.87	128.15	120.28
1	y	135	ILE	CA-C-N	5.87	128.07	120.44
1	y	135	ILE	C-N-CA	5.87	128.07	120.44
1	y	205	HIS	CE1-NE2-CD2	-5.87	103.14	109.00
14	4	2181	U	O5'-C5'-C4'	-5.87	102.70	111.50
9	U	11	ILE	N-CA-C	-5.85	107.05	113.43
1	y	61	ILE	O-C-N	5.85	127.64	121.91
2	E	96	ILE	N-CA-CB	5.84	117.39	110.55
14	4	2151	U	O4'-C4'-C3'	-5.84	98.16	104.00
5	p	19	G	P-O3'-C3'	5.83	128.95	120.20
1	y	434	LYS	CA-C-N	5.83	128.03	120.44
1	y	434	LYS	C-N-CA	5.83	128.03	120.44
14	4	2111	U	C4'-C3'-C2'	-5.83	96.77	102.60
1	y	300	TRP	CA-C-N	5.83	128.09	120.28
1	y	300	TRP	C-N-CA	5.83	128.09	120.28
1	y	64	PHE	N-CA-CB	-5.82	101.57	110.01
3	G	11	ILE	CA-C-N	5.82	127.89	120.56
3	G	11	ILE	C-N-CA	5.82	127.89	120.56
3	G	20	ILE	N-CA-C	5.82	116.47	110.36
3	G	43	PHE	O-C-N	-5.81	116.62	123.25
1	y	258	TYR	N-CA-CB	5.81	120.31	110.49
7	5	43	ASP	N-CA-C	-5.81	100.52	109.52
14	4	2164	C	C1'-O4'-C4'	-5.81	103.89	109.70
7	5	65	LEU	CA-C-O	-5.80	114.79	120.19
1	y	239	ARG	N-CA-CB	5.80	118.65	110.12
1	y	223	VAL	N-CA-C	5.80	116.54	110.62
2	E	97	VAL	O-C-N	5.80	127.50	121.87
1	y	137	THR	O-C-N	5.80	128.04	122.07
1	y	429	TYR	CA-C-O	-5.79	114.74	120.82
14	4	2177	C	C4'-C3'-C2'	-5.79	96.81	102.60
1	y	369	VAL	N-CA-CB	5.79	117.32	110.55
10	Y	51	ALA	CA-C-N	5.78	129.50	120.82
10	Y	51	ALA	C-N-CA	5.78	129.50	120.82
14	4	2177	C	O4'-C1'-N1	5.78	117.17	108.50
1	y	417	MET	N-CA-C	5.78	117.25	111.07
13	3	1518	C	C5'-C4'-C3'	5.77	124.66	116.00
5	p	14	A	C4'-C3'-C2'	-5.76	96.83	102.60
7	5	71	ARG	CD-NE-CZ	-5.76	116.33	124.40
7	5	48	LEU	N-CA-CB	5.76	119.80	110.41
7	5	8	MET	CA-C-N	5.76	127.92	120.44
7	5	8	MET	C-N-CA	5.76	127.92	120.44
5	p	6	A	P-O5'-C5'	-5.75	112.28	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	3	1540	G	P-O3'-C3'	-5.74	111.58	120.20
2	E	127	PHE	CB-CG-CD2	5.74	130.46	120.70
1	y	133	ILE	CA-C-N	5.74	126.31	119.94
1	y	133	ILE	C-N-CA	5.74	126.31	119.94
1	y	286	PHE	O-C-N	-5.74	115.37	120.48
4	n	8	LEU	N-CA-C	5.74	117.21	111.07
14	4	2137	U	C5'-C4'-O4'	5.73	118.40	109.80
1	y	390	PHE	CA-C-N	5.72	127.88	120.44
1	y	390	PHE	C-N-CA	5.72	127.88	120.44
7	5	71	ARG	NE-CZ-NH2	-5.72	114.06	119.20
1	y	427	SER	O-C-N	5.71	127.96	122.07
1	y	246	VAL	N-CA-CB	5.71	119.10	111.90
1	y	23	LEU	CA-C-N	5.71	127.86	120.44
1	y	23	LEU	C-N-CA	5.71	127.86	120.44
7	5	156	ALA	N-CA-CB	5.71	118.35	110.07
1	y	371	THR	O-C-N	5.70	127.94	122.07
1	y	219	VAL	CA-C-O	-5.69	115.03	120.95
1	y	273	GLY	CA-C-N	5.69	127.73	120.56
1	y	273	GLY	C-N-CA	5.69	127.73	120.56
5	p	31	C	O4'-C1'-N1	5.69	117.04	108.50
1	y	275	ILE	CA-C-N	5.68	124.88	118.97
1	y	275	ILE	C-N-CA	5.68	124.88	118.97
14	4	2116	G	C1'-O4'-C4'	-5.68	104.02	109.70
7	5	78	PHE	CB-CG-CD2	5.68	130.35	120.70
14	4	2162	G	O4'-C1'-N9	5.68	117.01	108.50
14	4	2091	C	O4'-C1'-N1	5.67	117.01	108.50
5	p	76	A	O4'-C1'-N9	5.67	117.00	108.50
1	y	381	ILE	N-CA-CB	5.66	116.80	110.51
1	y	284	ILE	CA-C-N	5.66	127.80	120.44
1	y	284	ILE	C-N-CA	5.66	127.80	120.44
1	y	151	ASN	O-C-N	5.66	126.67	121.80
14	4	2145	C	O4'-C1'-C2'	-5.66	100.14	105.80
1	y	31	ILE	CA-C-N	5.65	127.68	120.56
1	y	31	ILE	C-N-CA	5.65	127.68	120.56
1	y	59	THR	CA-C-N	5.65	127.68	120.56
1	y	59	THR	C-N-CA	5.65	127.68	120.56
7	5	1	MET	CG-SD-CE	-5.65	88.47	100.90
1	y	379	LEU	N-CA-C	5.65	117.11	111.07
14	4	2165	C	C4'-C3'-C2'	-5.65	96.95	102.60
7	5	152	ALA	CA-C-N	5.64	127.78	120.56
7	5	152	ALA	C-N-CA	5.64	127.78	120.56
14	4	2172	U	C5'-C4'-C3'	5.64	123.66	115.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	p	27	C	O3'-P-O5'	-5.64	95.55	104.00
13	3	1551	A	OP1-P-O3'	5.64	124.91	108.00
1	y	13	LYS	CA-C-N	5.63	126.23	119.98
1	y	13	LYS	C-N-CA	5.63	126.23	119.98
5	p	61	C	O4'-C1'-N1	5.63	116.94	108.50
1	y	372	ARG	CA-C-O	-5.63	114.91	120.82
14	4	2182	U	C4'-C3'-C2'	-5.62	96.98	102.60
6	a	10	G	C2'-C3'-O3'	5.61	122.12	113.70
14	4	2188	U	O4'-C4'-C3'	-5.61	98.39	104.00
1	y	365	TYR	CB-CG-CD1	5.61	129.22	120.80
14	4	2099	U	P-O5'-C5'	-5.61	112.49	120.90
14	4	2127	G	C5'-C4'-O4'	5.61	118.21	109.80
1	y	371	THR	CA-C-O	-5.61	114.93	120.82
2	E	86	THR	CB-CA-C	-5.60	102.08	110.88
10	Y	12	GLU	CA-C-N	5.60	127.79	120.28
10	Y	12	GLU	C-N-CA	5.60	127.79	120.28
14	4	2152	G	O5'-C5'-C4'	5.60	119.89	111.50
1	y	86	ILE	CA-C-O	-5.59	115.24	121.17
14	4	2150	C	P-O5'-C5'	-5.58	112.52	120.90
3	G	68	LEU	CB-CA-C	-5.58	101.53	110.79
1	y	300	TRP	CB-CG-CD1	-5.58	118.54	126.90
1	y	377	GLY	CA-C-N	5.57	127.68	120.44
1	y	377	GLY	C-N-CA	5.57	127.68	120.44
5	p	40	G	C2'-C3'-O3'	5.57	122.06	113.70
5	p	50	C	C1'-O4'-C4'	5.57	115.47	109.90
1	y	304	THR	CA-C-N	5.57	127.74	120.28
1	y	304	THR	C-N-CA	5.57	127.74	120.28
2	E	99	ALA	CA-C-N	5.56	128.08	120.46
2	E	99	ALA	C-N-CA	5.56	128.08	120.46
7	5	129	GLN	CG-CD-NE2	5.56	124.74	116.40
14	4	2092	U	C4'-C3'-O3'	5.56	117.74	109.40
14	4	2178	C	O4'-C1'-C2'	-5.56	102.04	107.60
7	5	18	THR	N-CA-C	-5.56	98.96	110.80
7	5	98	GLU	N-CA-C	-5.56	105.43	113.21
2	E	83	ILE	CA-CB-CG1	5.55	119.84	110.40
1	y	342	THR	N-CA-C	-5.55	105.13	111.07
7	5	176	GLY	CA-C-N	5.55	132.27	122.67
7	5	176	GLY	C-N-CA	5.55	132.27	122.67
1	y	196	VAL	CB-CA-C	-5.55	104.78	111.88
1	y	241	GLN	CA-C-O	-5.55	114.36	120.30
5	p	68	C	C5'-C4'-O4'	5.55	118.12	109.80
5	p	37	A	O5'-C5'-C4'	-5.54	103.18	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	4	2107	G	O3'-P-O5'	-5.54	95.69	104.00
7	5	212	VAL	CB-CA-C	5.54	118.37	110.84
1	y	25	PHE	CA-CB-CG	-5.54	108.26	113.80
1	y	111	SER	CB-CA-C	5.54	119.57	110.88
1	y	332	TYR	N-CA-CB	5.54	118.04	110.01
1	y	424	MET	CB-CA-C	-5.54	102.19	110.88
1	y	410	VAL	CA-C-N	5.53	127.53	120.56
1	y	410	VAL	C-N-CA	5.53	127.53	120.56
7	5	184	LYS	N-CA-CB	5.53	118.34	110.16
1	y	33	PHE	N-CA-C	5.52	116.98	111.07
14	4	2136	G	C4'-C3'-C2'	-5.52	97.08	102.60
1	y	218	LEU	N-CA-CB	5.52	118.01	110.01
5	p	69	C	C4'-C3'-O3'	-5.51	104.73	113.00
1	y	77	ILE	CB-CA-C	-5.51	103.63	111.40
4	n	46	ASP	N-CA-C	-5.51	99.06	110.80
1	y	344	ASP	CA-C-N	5.50	127.66	120.28
1	y	344	ASP	C-N-CA	5.50	127.66	120.28
1	y	57	ARG	N-CA-CB	5.50	119.79	110.49
1	y	413	ILE	CA-C-O	-5.50	115.34	121.17
1	y	116	ILE	N-CA-C	5.50	115.70	110.42
9	U	89	GLY	N-CA-C	-5.50	107.77	114.92
14	4	2148	G	P-O3'-C3'	5.50	128.44	120.20
1	y	429	TYR	O-C-N	5.49	127.73	122.07
1	y	327	PHE	O-C-N	5.49	127.72	122.07
4	n	22	TYR	O-C-N	-5.48	116.28	122.97
1	y	423	LEU	O-C-N	5.48	127.71	122.07
14	4	2132	U	C1'-O4'-C4'	-5.48	104.22	109.70
13	3	1530	G	O4'-C1'-N9	5.48	116.71	108.50
9	U	46	LYS	CA-C-N	5.47	125.48	119.90
9	U	46	LYS	C-N-CA	5.47	125.48	119.90
9	U	88	ASP	N-CA-C	-5.47	106.48	112.72
14	4	2164	C	P-O5'-C5'	-5.47	112.70	120.90
1	y	117	SER	N-CA-CB	5.46	118.15	110.12
7	5	78	PHE	CB-CG-CD1	-5.46	111.42	120.70
1	y	380	TYR	CA-C-O	-5.46	115.09	120.82
3	G	55	MET	N-CA-CB	5.46	117.93	110.01
7	5	139	ASN	CA-C-N	5.46	125.55	119.32
7	5	139	ASN	C-N-CA	5.46	125.55	119.32
14	4	2162	G	C1'-C2'-O2'	5.46	116.59	108.40
2	E	103	VAL	CA-C-N	5.46	127.53	120.44
2	E	103	VAL	C-N-CA	5.46	127.53	120.44
1	y	363	ALA	CA-C-N	5.46	127.53	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	y	363	ALA	C-N-CA	5.46	127.53	120.44
2	E	97	VAL	CA-C-N	5.45	127.53	120.44
2	E	97	VAL	C-N-CA	5.45	127.53	120.44
1	y	29	ALA	N-CA-C	5.45	116.90	111.07
14	4	2198	A	O3'-P-O5'	-5.45	95.83	104.00
3	G	9	PHE	CA-CB-CG	-5.45	108.36	113.80
7	5	188	ASN	CA-C-N	5.44	127.52	120.44
7	5	188	ASN	C-N-CA	5.44	127.52	120.44
1	y	14	GLY	N-CA-C	-5.44	106.20	112.73
7	5	15	VAL	N-CA-CB	5.44	118.31	111.46
14	4	2120	G	C5'-C4'-C3'	5.44	124.16	116.00
7	5	118	PRO	N-CA-CB	5.43	108.95	103.25
1	y	195	ILE	N-CA-CB	5.42	116.90	110.55
5	p	43	G	O4'-C1'-C2'	-5.42	102.17	107.60
1	y	180	GLU	CB-CG-CD	5.42	121.82	112.60
1	y	389	GLU	CA-C-N	5.42	127.48	120.44
1	y	389	GLU	C-N-CA	5.42	127.48	120.44
7	5	47	ASN	CB-CG-ND2	-5.42	108.27	116.40
1	y	145	MET	CA-C-N	5.41	131.47	121.94
1	y	145	MET	C-N-CA	5.41	131.47	121.94
5	p	4	G	P-O5'-C5'	5.41	129.02	120.90
13	3	1535	A	O4'-C1'-N9	5.41	116.32	108.20
1	y	424	MET	N-CA-C	5.41	116.85	111.07
3	G	61	THR	N-CA-CB	5.41	117.85	110.01
1	y	75	ALA	N-CA-C	-5.40	104.03	110.41
1	y	335	LEU	N-CA-C	5.40	116.85	111.07
6	a	9	A	N9-C1'-C2'	5.40	120.10	112.00
5	p	55	U	O4'-C4'-C3'	-5.39	98.61	104.00
1	y	27	ILE	N-CA-C	-5.39	105.24	110.42
14	4	2095	A	C5'-C4'-C3'	-5.39	107.91	116.00
14	4	2130	U	C5'-C4'-O4'	5.39	117.88	109.80
14	4	2111	U	C4'-C3'-O3'	-5.39	104.92	113.00
1	y	331	PHE	N-CA-C	5.39	116.83	111.07
1	y	386	LEU	N-CA-CB	5.39	118.04	110.12
7	5	126	GLN	CA-C-N	5.39	129.34	121.31
7	5	126	GLN	C-N-CA	5.39	129.34	121.31
7	5	164	ARG	CG-CD-NE	-5.38	100.16	112.00
1	y	374	THR	CB-CA-C	5.38	119.72	110.79
7	5	160	GLN	CA-C-O	-5.38	114.83	120.80
1	y	223	VAL	CA-CB-CG1	5.38	119.54	110.40
1	y	22	ARG	NH1-CZ-NH2	-5.38	112.31	119.30
1	y	96	THR	N-CA-C	5.37	117.13	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	y	394	ALA	N-CA-C	5.37	116.81	111.07
1	y	329	CYS	CA-C-N	5.37	127.41	120.44
1	y	329	CYS	C-N-CA	5.37	127.41	120.44
1	y	228	PHE	CA-C-N	5.36	127.41	120.44
1	y	228	PHE	C-N-CA	5.36	127.41	120.44
3	G	69	VAL	O-C-N	5.36	127.17	121.91
1	y	22	ARG	N-CA-C	5.36	117.12	111.28
7	5	51	ASP	N-CA-C	-5.36	106.42	113.17
14	4	2104	C	O4'-C1'-N1	5.36	116.54	108.50
14	4	2151	U	O4'-C1'-N1	5.36	116.53	108.50
1	y	33	PHE	CA-CB-CG	-5.35	108.45	113.80
1	y	415	ASP	CB-CA-C	-5.35	102.48	110.88
1	y	232	PHE	O-C-N	5.35	127.58	122.07
5	p	22	G	O3'-P-O5'	-5.35	95.98	104.00
7	5	182	ALA	CA-C-N	5.34	127.88	120.29
7	5	182	ALA	C-N-CA	5.34	127.88	120.29
7	5	51	ASP	CA-CB-CG	5.34	117.94	112.60
3	G	26	LYS	CB-CA-C	-5.34	102.50	110.88
7	5	63	THR	CA-C-N	5.34	129.27	121.80
7	5	63	THR	C-N-CA	5.34	129.27	121.80
7	5	117	SER	N-CA-C	-5.34	102.06	108.25
14	4	2154	A	O4'-C1'-N9	5.33	116.50	108.50
1	y	340	ARG	NH1-CZ-NH2	-5.33	112.37	119.30
7	5	40	GLU	N-CA-CB	5.33	119.58	110.57
1	y	230	VAL	CB-CA-C	-5.33	105.15	111.97
2	E	81	LYS	CA-C-N	5.33	127.76	120.46
2	E	81	LYS	C-N-CA	5.33	127.76	120.46
1	y	373	LEU	CA-C-N	5.33	127.42	120.28
1	y	373	LEU	C-N-CA	5.33	127.42	120.28
7	5	155	ASN	CA-C-N	5.33	127.68	120.44
7	5	155	ASN	C-N-CA	5.33	127.68	120.44
4	n	8	LEU	CA-C-N	5.32	127.36	120.44
4	n	8	LEU	C-N-CA	5.32	127.36	120.44
5	p	6	A	P-O3'-C3'	5.32	128.18	120.20
5	p	42	C	P-O5'-C5'	-5.32	112.92	120.90
1	y	50	ALA	N-CA-CB	5.31	117.71	110.01
1	y	355	GLY	N-CA-C	-5.31	108.02	114.92
14	4	2141	G	C5'-C4'-C3'	-5.31	108.04	116.00
1	y	175	GLY	CA-C-N	5.30	127.39	120.28
1	y	175	GLY	C-N-CA	5.30	127.39	120.28
1	y	234	VAL	O-C-N	5.30	127.11	121.91
14	4	2180	U	O4'-C1'-C2'	-5.29	102.31	107.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	y	88	ALA	CA-C-N	5.29	127.37	120.28
1	y	88	ALA	C-N-CA	5.29	127.37	120.28
7	5	43	ASP	CA-CB-CG	5.29	117.89	112.60
1	y	374	THR	O-C-N	-5.29	116.51	122.12
1	y	386	LEU	N-CA-C	5.29	117.05	111.28
3	G	32	ALA	CA-C-N	5.29	127.36	120.28
3	G	32	ALA	C-N-CA	5.29	127.36	120.28
14	4	2099	U	C2'-C3'-O3'	5.29	121.63	113.70
7	5	171	ILE	N-CA-C	-5.29	99.34	106.85
7	5	67	HIS	CA-CB-CG	5.28	119.08	113.80
14	4	2093	G	P-O3'-C3'	-5.28	112.28	120.20
7	5	166	ASP	CA-C-N	5.28	127.35	120.28
7	5	166	ASP	C-N-CA	5.28	127.35	120.28
7	5	102	ASP	O-C-N	5.27	127.58	122.09
7	5	153	VAL	N-CA-C	-5.27	105.58	110.53
14	4	2164	C	P-O3'-C3'	5.27	128.10	120.20
1	y	192	PHE	CA-CB-CG	-5.26	108.53	113.80
14	4	2198	A	O4'-C1'-N9	5.26	116.09	108.20
2	E	94	THR	CA-C-O	-5.26	114.95	120.63
2	E	97	VAL	CA-C-O	-5.26	115.48	120.95
7	5	163	TYR	N-CA-C	-5.26	101.19	109.50
14	4	2160	C	O4'-C1'-N1	5.26	116.39	108.50
1	y	324	ALA	CA-C-N	5.25	127.18	120.56
1	y	324	ALA	C-N-CA	5.25	127.18	120.56
14	4	2147	A	C2'-C3'-O3'	5.25	121.57	113.70
1	y	357	ARG	N-CA-CB	5.25	117.67	110.01
4	n	17	ALA	N-CA-CB	5.24	119.35	110.49
3	G	21	MET	CA-C-N	5.24	127.25	120.44
3	G	21	MET	C-N-CA	5.24	127.25	120.44
7	5	114	VAL	N-CA-C	-5.24	99.70	107.51
1	y	203	ILE	CA-C-N	5.24	127.25	120.44
1	y	203	ILE	C-N-CA	5.24	127.25	120.44
1	y	107	LYS	N-CA-CB	5.24	117.60	110.01
1	y	408	ILE	CA-C-N	5.23	127.15	120.56
1	y	408	ILE	C-N-CA	5.23	127.15	120.56
1	y	119	TYR	CB-CG-CD2	-5.22	112.96	120.80
1	y	279	PHE	O-C-N	5.22	127.45	122.07
14	4	2182	U	O3'-P-O5'	-5.22	96.17	104.00
1	y	115	LYS	N-CA-CB	5.22	117.58	110.01
13	3	1533	C	P-O5'-C5'	5.22	128.73	120.90
14	4	2092	U	C5'-C4'-C3'	-5.22	107.37	115.20
14	4	2135	A	C4'-C3'-O3'	-5.21	105.18	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	y	103	ALA	CA-C-N	5.21	127.57	120.54
1	y	103	ALA	C-N-CA	5.21	127.57	120.54
2	E	93	THR	CA-C-O	-5.21	114.37	120.20
14	4	2169	A	O4'-C1'-N9	5.20	116.31	108.50
1	y	127	LEU	O-C-N	5.20	127.43	122.07
1	y	165	VAL	N-CA-C	5.20	115.92	110.62
1	y	267	LEU	CB-CA-C	5.20	119.96	111.23
1	y	32	VAL	O-C-N	-5.20	116.82	121.91
7	5	47	ASN	CB-CG-OD1	5.20	131.19	120.80
7	5	50	ILE	N-CA-CB	5.20	117.38	110.26
4	n	1	ALA	CA-C-N	5.19	127.49	120.38
4	n	1	ALA	C-N-CA	5.19	127.49	120.38
1	y	151	ASN	N-CA-C	-5.19	101.12	109.58
2	E	80	ARG	N-CA-C	5.19	116.62	111.07
2	E	91	LEU	N-CA-CB	5.19	118.25	110.11
5	p	52	A	C1'-C2'-O2'	5.19	116.18	108.40
14	4	2194	U	C3'-C2'-O2'	5.18	118.47	110.70
1	y	107	LYS	N-CA-C	5.18	116.61	111.07
7	5	139	ASN	N-CA-C	-5.18	99.84	109.06
2	E	78	GLU	N-CA-C	-5.18	105.64	111.28
1	y	138	GLY	N-CA-C	5.17	118.50	112.50
14	4	2101	A	O4'-C1'-N9	5.17	116.26	108.50
1	y	383	PHE	CA-C-N	5.16	127.06	120.56
1	y	383	PHE	C-N-CA	5.16	127.06	120.56
7	5	210	LYS	CA-C-N	5.16	128.67	121.24
7	5	210	LYS	C-N-CA	5.16	128.67	121.24
13	3	1535	A	O4'-C1'-C2'	-5.16	100.64	105.80
1	y	53	LEU	O-C-N	5.16	127.38	122.07
3	G	58	LEU	CA-C-N	5.15	127.49	120.54
3	G	58	LEU	C-N-CA	5.15	127.49	120.54
14	4	2124	G	O4'-C1'-N9	5.15	116.22	108.50
2	E	112	ASP	CA-C-N	-5.15	114.23	119.94
2	E	112	ASP	C-N-CA	-5.15	114.23	119.94
14	4	2121	G	C4'-C3'-O3'	-5.14	105.29	113.00
1	y	279	PHE	CA-CB-CG	5.14	118.94	113.80
1	y	430	GLU	N-CA-C	5.14	116.57	111.07
5	p	65	U	C4'-C3'-O3'	-5.13	105.30	113.00
14	4	2101	A	O3'-P-O5'	-5.13	96.30	104.00
1	y	395	MET	N-CA-C	5.13	116.87	111.28
1	y	248	TYR	CA-C-N	5.13	131.33	121.54
1	y	248	TYR	C-N-CA	5.13	131.33	121.54
1	y	437	ASN	CA-CB-CG	5.13	117.73	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	77	THR	O-C-N	5.12	127.35	122.07
7	5	157	LYS	CA-C-N	5.12	127.10	120.44
7	5	157	LYS	C-N-CA	5.12	127.10	120.44
4	n	11	LEU	CA-C-N	5.12	127.01	120.56
4	n	11	LEU	C-N-CA	5.12	127.01	120.56
5	p	67	U	O4'-C1'-N1	5.12	116.18	108.50
14	4	2105	U	C4'-C3'-O3'	-5.12	105.32	113.00
3	G	65	ILE	O-C-N	-5.12	116.83	121.94
14	4	2141	G	C1'-C2'-O2'	5.12	116.07	108.40
1	y	412	VAL	CA-CB-CG1	5.11	119.09	110.40
7	5	211	LYS	N-CA-CB	5.11	117.59	109.71
1	y	25	PHE	CA-C-N	5.11	127.00	120.56
1	y	25	PHE	C-N-CA	5.11	127.00	120.56
13	3	1515	A	O4'-C1'-N9	5.11	116.16	108.50
1	y	327	PHE	CA-C-N	5.11	127.08	120.44
1	y	327	PHE	C-N-CA	5.11	127.08	120.44
1	y	40	PRO	N-CA-CB	5.10	108.61	103.25
1	y	87	SER	CA-C-N	5.10	127.07	120.44
1	y	87	SER	C-N-CA	5.10	127.07	120.44
1	y	328	PHE	CA-CB-CG	-5.10	108.70	113.80
14	4	2192	U	O4'-C1'-N1	5.10	116.15	108.50
1	y	232	PHE	N-CA-CB	-5.10	102.61	110.01
1	y	390	PHE	CA-CB-CG	-5.10	108.70	113.80
2	E	82	VAL	CA-CB-CG2	-5.10	101.74	110.40
1	y	162	VAL	CA-C-O	5.09	126.57	121.17
1	y	345	ASN	N-CA-CB	5.09	117.60	110.12
1	y	345	ASN	N-CA-C	5.09	116.83	111.28
1	y	379	LEU	O-C-N	5.09	127.31	122.07
5	p	40	G	C5'-C4'-C3'	-5.09	108.37	116.00
1	y	208	GLU	CA-C-N	5.08	127.40	120.54
1	y	208	GLU	C-N-CA	5.08	127.40	120.54
2	E	84	TRP	CA-C-O	-5.08	113.75	118.73
9	U	24	VAL	CA-C-N	5.08	127.39	120.54
9	U	24	VAL	C-N-CA	5.08	127.39	120.54
7	5	154	LYS	CA-C-O	5.08	126.61	120.92
12	2	1324	G	C5'-C4'-C3'	-5.08	107.59	115.20
1	y	165	VAL	CA-CB-CG1	5.07	119.03	110.40
3	G	35	GLY	CA-C-N	5.07	131.06	122.79
3	G	35	GLY	C-N-CA	5.07	131.06	122.79
13	3	1517	G	C5'-C4'-C3'	5.07	123.61	116.00
3	G	52	MET	CA-C-N	5.07	127.07	120.28
3	G	52	MET	C-N-CA	5.07	127.07	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	y	113	ARG	NE-CZ-NH1	5.07	126.57	121.50
5	p	14	A	P-O5'-C5'	-5.07	113.30	120.90
1	y	354	PRO	O-C-N	-5.07	117.18	123.01
3	G	41	THR	CA-CB-CG2	-5.06	101.90	110.50
5	p	30	C	C1'-O4'-C4'	5.06	114.96	109.90
5	p	14	A	C4'-C3'-O3'	-5.05	105.42	113.00
14	4	2117	A	C3'-C2'-O2'	5.05	118.28	110.70
14	4	2118	U	C4'-C3'-C2'	5.05	107.65	102.60
1	y	341	GLU	CB-CA-C	-5.05	102.95	110.88
7	5	112	ASP	N-CA-C	-5.05	105.43	112.45
5	p	23	A	C4'-C3'-O3'	-5.05	105.43	113.00
5	p	49	G	O4'-C1'-N9	5.05	116.07	108.50
1	y	209	GLN	N-CA-CB	5.05	117.46	109.94
3	G	64	PHE	CA-C-N	5.05	127.11	120.60
3	G	64	PHE	C-N-CA	5.05	127.11	120.60
10	Y	4	LYS	CA-C-N	5.05	127.35	120.54
10	Y	4	LYS	C-N-CA	5.05	127.35	120.54
1	y	127	LEU	CA-C-O	-5.04	115.53	120.82
7	5	145	VAL	N-CA-C	-5.04	108.38	113.47
14	4	2141	G	C5'-C4'-O4'	5.04	117.36	109.80
14	4	2097	A	O4'-C1'-N9	5.04	116.06	108.50
5	p	43	G	O4'-C1'-N9	5.03	116.05	108.50
5	p	44	G	C5'-C4'-O4'	5.03	117.35	109.80
5	p	24	G	C4'-C3'-C2'	-5.03	97.57	102.60
1	y	67	PHE	CB-CA-C	-5.03	102.98	110.88
14	4	2158	A	P-O5'-C5'	5.03	128.44	120.90
3	G	56	THR	CA-C-N	5.03	126.97	120.44
3	G	56	THR	C-N-CA	5.03	126.97	120.44
1	y	274	VAL	CA-C-N	5.03	124.35	120.33
1	y	274	VAL	C-N-CA	5.03	124.35	120.33
1	y	374	THR	CA-C-N	5.02	127.01	120.28
1	y	374	THR	C-N-CA	5.02	127.01	120.28
14	4	2103	C	P-O5'-C5'	5.02	128.43	120.90
1	y	254	GLY	O-C-N	5.02	129.22	122.70
3	G	11	ILE	CA-CB-CG1	5.01	118.92	110.40
1	y	394	ALA	N-CA-CB	5.01	117.28	110.01
1	y	19	LEU	N-CA-C	5.01	116.74	111.28
1	y	130	PHE	O-C-N	5.01	127.30	122.09
1	y	427	SER	N-CA-C	5.01	116.43	111.07
14	4	2183	A	P-O5'-C5'	-5.01	113.39	120.90
3	G	32	ALA	O-C-N	5.00	127.49	122.09
7	5	65	LEU	N-CA-C	-5.00	103.41	110.31

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	y	55	GLN	CA
1	y	56	GLN	CA
4	n	38	LEU	CA
4	n	39	HIS	CA
4	n	40	GLN	CA

All (141) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	1	60	G	Sidechain
11	1	72	U	Sidechain
12	2	1327	A	Sidechain
12	2	1334	G	Sidechain
13	3	1515	A	Sidechain
13	3	1517	G	Sidechain
13	3	1519	G	Sidechain
13	3	1520	U	Sidechain
13	3	1521	G	Sidechain
13	3	1522	A	Sidechain
13	3	1523	U	Sidechain
13	3	1524	G	Sidechain
13	3	1525	A	Sidechain
13	3	1529	G	Sidechain
13	3	1530	G	Sidechain
13	3	1531	C	Sidechain
13	3	1533	C	Sidechain
13	3	1536	C	Sidechain
13	3	1539	U	Sidechain
13	3	1540	G	Sidechain
13	3	1545	A	Sidechain
13	3	1546	G	Sidechain
13	3	1550	C	Sidechain
14	4	2099	U	Sidechain
14	4	2100	G	Sidechain
14	4	2101	A	Sidechain
14	4	2104	C	Sidechain
14	4	2105	U	Sidechain
14	4	2106	U	Sidechain
14	4	2107	G	Sidechain
14	4	2108	A	Sidechain
14	4	2110	G	Sidechain
14	4	2112	G	Sidechain

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Mol	Chain	Res	Type	Group
14	4	2113	U	Sidechain
14	4	2115	G	Sidechain
14	4	2116	G	Sidechain
14	4	2118	U	Sidechain
14	4	2119	A	Sidechain
14	4	2120	G	Sidechain
14	4	2123	G	Sidechain
14	4	2124	G	Sidechain
14	4	2125	G	Sidechain
14	4	2126	A	Sidechain
14	4	2127	G	Sidechain
14	4	2128	G	Sidechain
14	4	2129	C	Sidechain
14	4	2133	G	Sidechain
14	4	2135	A	Sidechain
14	4	2136	G	Sidechain
14	4	2140	G	Sidechain
14	4	2142	A	Sidechain
14	4	2144	G	Sidechain
14	4	2148	G	Sidechain
14	4	2149	U	Sidechain
14	4	2150	C	Sidechain
14	4	2152	G	Sidechain
14	4	2153	C	Sidechain
14	4	2154	A	Sidechain
14	4	2155	U	Sidechain
14	4	2156	G	Sidechain
14	4	2157	G	Sidechain
14	4	2159	G	Sidechain
14	4	2160	C	Sidechain
14	4	2161	C	Sidechain
14	4	2167	U	Sidechain
14	4	2168	G	Sidechain
14	4	2169	A	Sidechain
14	4	2172	U	Sidechain
14	4	2173	A	Sidechain
14	4	2174	C	Sidechain
14	4	2175	C	Sidechain
14	4	2176	A	Sidechain
14	4	2177	C	Sidechain
14	4	2179	C	Sidechain
14	4	2182	U	Sidechain

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Mol	Chain	Res	Type	Group
14	4	2183	A	Sidechain
14	4	2184	A	Sidechain
14	4	2185	U	Sidechain
14	4	2186	G	Sidechain
14	4	2187	U	Sidechain
14	4	2189	U	Sidechain
14	4	2190	G	Sidechain
14	4	2192	U	Sidechain
14	4	2194	U	Sidechain
14	4	2196	C	Sidechain
14	4	2197	U	Sidechain
7	5	122	ARG	Sidechain
7	5	163	TYR	Sidechain
7	5	208	TYR	Sidechain
2	E	87	ARG	Sidechain
2	E	93	THR	Mainchain
3	G	41	THR	Peptide
9	U	48	VAL	Peptide
6	a	66	U	Sidechain
5	p	1	G	Sidechain
5	p	13	C	Sidechain
5	p	24	G	Sidechain
5	p	26	A	Sidechain
5	p	27	C	Sidechain
5	p	28	G	Sidechain
5	p	29	A	Sidechain
5	p	3	G	Sidechain
5	p	31	C	Sidechain
5	p	33	U	Sidechain
5	p	34	G	Sidechain
5	p	36	C	Sidechain
5	p	38	A	Sidechain
5	p	39	G	Sidechain
5	p	40	G	Sidechain
5	p	41	U	Sidechain
5	p	44	G	Sidechain
5	p	45	G	Sidechain
5	p	48	C	Sidechain
5	p	49	G	Sidechain
5	p	53	G	Sidechain
5	p	55	U	Sidechain
5	p	58	A	Sidechain

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Mol	Chain	Res	Type	Group
5	p	63	C	Sidechain
5	p	65	U	Sidechain
5	p	69	C	Sidechain
5	p	70	C	Sidechain
5	p	74	C	Sidechain
5	p	76	A	Sidechain
1	y	22	ARG	Sidechain
1	y	232	PHE	Sidechain
1	y	243	ARG	Sidechain
1	y	248	TYR	Sidechain
1	y	265	LEU	Peptide
1	y	266	PRO	Mainchain
1	y	309	TYR	Sidechain
1	y	321	TYR	Sidechain
1	y	332	TYR	Sidechain
1	y	34	ARG	Sidechain
1	y	357	ARG	Sidechain
1	y	365	TYR	Sidechain
1	y	38	PHE	Sidechain
1	y	424	MET	Mainchain
1	y	45	ASP	Sidechain
1	y	57	ARG	Sidechain
1	y	67	PHE	Sidechain
1	y	85	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	y	3361	0	3514	284	0
2	E	433	0	466	31	0
3	G	461	0	485	22	0
4	n	760	0	742	376	0
5	p	1621	0	818	10	0
6	a	1626	0	833	74	0
7	5	1733	0	1824	8	0
8	T	787	0	844	35	0
9	U	789	0	847	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	Y	509	0	543	6	0
11	1	1350	0	678	37	0
12	2	775	0	389	13	0
13	3	948	0	478	0	0
14	4	2325	0	1168	8	0
All	All	17478	0	13629	610	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 20.

All (610) 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)
2:E:81:LYS:HD2	8:T:93:LEU:CD1	1.30	1.62
1:y:52:LEU:HB2	4:n:29:GLU:CB	1.23	1.58
1:y:52:LEU:CB	4:n:29:GLU:HB3	1.36	1.52
2:E:81:LYS:CD	8:T:93:LEU:HD12	1.04	1.51
1:y:253:GLN:HB3	11:1:91:A:N6	1.27	1.43
4:n:85:PHE:CD1	4:n:87:THR:HG23	1.51	1.42
1:y:293:TRP:CZ2	4:n:22:TYR:CD2	2.12	1.38
1:y:256:ARG:O	11:1:92:U:C2	1.75	1.37
1:y:293:TRP:NE1	4:n:22:TYR:HD2	1.23	1.37
1:y:293:TRP:CE2	4:n:22:TYR:CD2	2.12	1.36
1:y:256:ARG:C	11:1:92:U:O2	1.68	1.36
1:y:293:TRP:CE2	4:n:22:TYR:HD2	1.41	1.34
4:n:22:TYR:C	4:n:23:GLU:N	1.84	1.33
1:y:52:LEU:CB	4:n:29:GLU:CB	1.95	1.32
1:y:253:GLN:CB	11:1:91:A:N6	1.93	1.31
4:n:61:LYS:O	4:n:62:MET:HG2	1.21	1.31
4:n:32:ARG:CG	4:n:33:GLN:H	1.42	1.30
4:n:85:PHE:CD1	4:n:87:THR:CG2	2.13	1.29
4:n:99:ALA:C	4:n:100:GLY:N	1.89	1.29
1:y:293:TRP:NE1	4:n:22:TYR:CD2	2.02	1.27
1:y:253:GLN:HB3	11:1:91:A:C6	1.70	1.26
1:y:253:GLN:CB	11:1:91:A:C6	2.19	1.25
1:y:365:TYR:OH	8:T:22:THR:OG1	1.53	1.23
2:E:81:LYS:CD	8:T:93:LEU:CD1	1.94	1.21
4:n:72:ALA:HA	4:n:76:VAL:CG2	1.73	1.19
1:y:293:TRP:CE2	4:n:22:TYR:HB2	1.79	1.17
2:E:81:LYS:HZ3	8:T:93:LEU:CG	1.57	1.17
1:y:16:LEU:HD11	4:n:53:TYR:OH	1.45	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:52:LEU:CB	4:n:29:GLU:CG	2.24	1.16
1:y:418:ALA:CB	4:n:41:ARG:O	1.91	1.16
1:y:275:ILE:HD12	4:n:6:LEU:HD11	1.19	1.16
1:y:254:GLY:HA2	11:1:91:A:N9	1.58	1.16
1:y:145:MET:SD	4:n:30:LEU:HD21	1.85	1.15
4:n:23:GLU:HG3	4:n:29:GLU:O	1.47	1.15
1:y:52:LEU:HB2	4:n:29:GLU:CG	1.76	1.14
1:y:16:LEU:HD21	4:n:53:TYR:CE2	1.83	1.14
1:y:185:ASN:HB3	4:n:39:HIS:HE1	1.07	1.14
4:n:32:ARG:O	4:n:33:GLN:HG2	1.47	1.13
2:E:81:LYS:CE	8:T:93:LEU:HD12	1.77	1.13
1:y:145:MET:O	4:n:30:LEU:HD22	1.46	1.12
1:y:275:ILE:CD1	4:n:6:LEU:HD11	1.78	1.12
4:n:85:PHE:CE1	4:n:87:THR:CG2	2.32	1.12
2:E:81:LYS:NZ	8:T:93:LEU:HG	1.65	1.12
1:y:425:MET:HE3	4:n:47:GLY:HA2	1.29	1.11
4:n:51:HIS:O	4:n:52:SER:HB3	1.44	1.11
2:E:81:LYS:NZ	8:T:93:LEU:CD1	2.13	1.11
1:y:12:ALA:CB	4:n:52:SER:HA	1.80	1.10
1:y:257:VAL:HG21	11:1:93:G:N2	1.66	1.10
4:n:32:ARG:HG3	4:n:33:GLN:N	1.38	1.10
4:n:61:LYS:O	4:n:62:MET:CG	1.99	1.10
1:y:52:LEU:HB2	4:n:29:GLU:HB2	1.28	1.10
4:n:72:ALA:HA	4:n:76:VAL:HG21	1.33	1.10
6:a:74:C:O2'	6:a:75:C:H5'	1.48	1.10
2:E:81:LYS:HD3	8:T:93:LEU:HB2	1.26	1.10
4:n:72:ALA:CA	4:n:76:VAL:CG2	2.30	1.09
1:y:365:TYR:CZ	8:T:22:THR:OG1	2.06	1.09
1:y:418:ALA:HB3	4:n:41:ARG:O	1.49	1.08
1:y:279:PHE:HA	4:n:13:LEU:HD13	1.10	1.08
1:y:293:TRP:CD2	4:n:22:TYR:HB2	1.88	1.08
1:y:52:LEU:HA	4:n:29:GLU:HG3	1.35	1.07
1:y:415:ASP:HA	4:n:41:ARG:CB	1.83	1.07
1:y:185:ASN:HB3	4:n:39:HIS:CE1	1.91	1.05
4:n:62:MET:HG3	9:U:51:LEU:HD23	1.38	1.05
4:n:72:ALA:CA	4:n:76:VAL:HG21	1.87	1.05
1:y:185:ASN:CB	4:n:39:HIS:HE1	1.70	1.04
1:y:257:VAL:HG21	11:1:93:G:C2	1.92	1.04
1:y:356:ILE:HA	8:T:18:GLU:HB3	1.38	1.04
1:y:52:LEU:HB3	4:n:29:GLU:HB3	1.32	1.04
1:y:279:PHE:CA	4:n:13:LEU:HD13	1.86	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:425:MET:CE	4:n:47:GLY:HA3	1.88	1.04
4:n:62:MET:CG	9:U:51:LEU:HD23	1.88	1.03
1:y:253:GLN:HB2	11:1:91:A:C6	1.89	1.03
4:n:63:THR:HG22	4:n:64:LYS:N	1.67	1.03
1:y:425:MET:HE3	4:n:47:GLY:CA	1.87	1.03
2:E:81:LYS:HZ2	8:T:93:LEU:CD1	1.71	1.03
4:n:85:PHE:HD1	4:n:87:THR:CG2	1.59	1.02
4:n:73:VAL:HG11	12:2:1322:A:O2'	1.60	1.02
4:n:73:VAL:CG1	12:2:1322:A:O2'	2.07	1.02
1:y:257:VAL:CG2	11:1:93:G:C2	2.43	1.02
1:y:415:ASP:HA	4:n:41:ARG:HB2	1.05	1.02
1:y:254:GLY:HA2	11:1:91:A:C4	1.95	1.01
3:G:41:THR:HG21	4:n:40:GLN:HE22	1.24	1.01
4:n:63:THR:HG22	4:n:64:LYS:H	0.85	1.01
4:n:73:VAL:HG13	4:n:74:ALA:HA	1.42	1.01
1:y:52:LEU:CA	4:n:29:GLU:HG3	1.90	1.01
2:E:81:LYS:HD3	8:T:93:LEU:CB	1.91	1.01
4:n:63:THR:CG2	4:n:64:LYS:H	1.71	1.01
4:n:73:VAL:HG22	4:n:77:ALA:HB2	1.39	1.00
4:n:11:LEU:CD1	4:n:36:PHE:CE1	2.45	1.00
1:y:52:LEU:CB	4:n:29:GLU:HG3	1.91	1.00
4:n:11:LEU:HD12	4:n:36:PHE:CE1	1.98	0.99
4:n:72:ALA:CB	4:n:76:VAL:HG21	1.92	0.99
1:y:253:GLN:HB2	11:1:91:A:N1	1.78	0.98
1:y:254:GLY:HA2	11:1:91:A:C8	1.97	0.98
2:E:81:LYS:NZ	8:T:93:LEU:CG	2.22	0.98
1:y:83:MET:HB2	4:n:36:PHE:HB2	1.46	0.98
4:n:72:ALA:HB1	4:n:76:VAL:CB	1.95	0.96
1:y:139:LEU:HD21	4:n:33:GLN:HG2	1.47	0.96
1:y:145:MET:SD	4:n:30:LEU:CD2	2.53	0.96
4:n:85:PHE:CE1	4:n:87:THR:HG23	1.97	0.96
1:y:425:MET:CE	4:n:47:GLY:CA	2.43	0.96
4:n:32:ARG:CG	4:n:33:GLN:N	2.12	0.96
4:n:59:GLY:O	4:n:60:VAL:HB	1.63	0.96
2:E:81:LYS:HZ3	8:T:93:LEU:HG	0.81	0.96
4:n:37:ALA:O	4:n:38:LEU:HB2	1.63	0.95
4:n:72:ALA:HB1	4:n:76:VAL:HB	1.48	0.94
1:y:252:GLN:HE22	8:T:70:HIS:CG	1.84	0.94
1:y:279:PHE:HA	4:n:13:LEU:CD1	1.97	0.94
4:n:73:VAL:CG2	4:n:77:ALA:HB2	1.98	0.94
1:y:419:GLN:HE22	4:n:3:LYS:NZ	1.65	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:81:LYS:HZ2	8:T:93:LEU:HD11	1.32	0.94
1:y:415:ASP:HB2	4:n:39:HIS:HD2	1.31	0.94
1:y:16:LEU:HD21	4:n:53:TYR:CZ	2.03	0.93
4:n:52:SER:OG	4:n:55:SER:HB3	1.68	0.93
4:n:72:ALA:HA	4:n:76:VAL:HG23	1.50	0.93
2:E:81:LYS:HD3	8:T:93:LEU:HD12	1.50	0.93
3:G:41:THR:CG2	4:n:40:GLN:HE22	1.79	0.93
4:n:85:PHE:CE1	4:n:87:THR:HG21	2.03	0.93
1:y:415:ASP:CA	4:n:41:ARG:HB2	1.96	0.93
1:y:16:LEU:CD2	4:n:53:TYR:CE2	2.51	0.93
4:n:32:ARG:O	4:n:33:GLN:CG	2.17	0.93
4:n:23:GLU:CG	4:n:29:GLU:O	2.16	0.92
4:n:32:ARG:NH1	4:n:34:HIS:ND1	2.16	0.92
4:n:55:SER:C	4:n:56:LEU:HD23	1.95	0.92
1:y:52:LEU:CG	4:n:29:GLU:HB3	2.00	0.92
1:y:257:VAL:HA	11:1:92:U:H3	1.33	0.92
4:n:23:GLU:O	4:n:24:ASP:HB2	1.69	0.92
1:y:293:TRP:CE2	4:n:22:TYR:CB	2.52	0.91
6:a:69:G:H2'	6:a:70:G:H5''	1.49	0.91
4:n:100:GLY:C	5:p:76:A:O3'	2.13	0.91
4:n:32:ARG:HH11	4:n:34:HIS:HA	1.34	0.91
1:y:8:ASP:HB3	4:n:54:HIS:O	1.69	0.90
4:n:64:LYS:HG2	4:n:65:TYR:N	1.83	0.90
6:a:74:C:O2'	6:a:75:C:C5'	2.20	0.89
1:y:425:MET:HE1	4:n:47:GLY:HA3	1.54	0.89
6:a:7:A:H5'	6:a:8:U:OP2	1.71	0.88
1:y:145:MET:C	4:n:30:LEU:HD22	2.00	0.87
1:y:145:MET:O	4:n:30:LEU:CD2	2.21	0.87
4:n:72:ALA:CA	4:n:76:VAL:HG23	2.01	0.87
1:y:293:TRP:HZ2	4:n:22:TYR:CD2	1.81	0.87
1:y:293:TRP:CE2	4:n:22:TYR:CG	2.62	0.87
1:y:419:GLN:HE22	4:n:3:LYS:CE	1.89	0.86
1:y:56:GLN:O	1:y:61:ILE:HG21	1.75	0.85
4:n:55:SER:C	4:n:56:LEU:CD2	2.48	0.85
1:y:257:VAL:HB	11:1:93:G:N3	1.92	0.85
1:y:12:ALA:CB	4:n:52:SER:CA	2.54	0.85
1:y:415:ASP:HB2	4:n:39:HIS:CD2	2.11	0.85
1:y:254:GLY:CA	11:1:91:A:C4	2.59	0.85
2:E:81:LYS:HD2	8:T:93:LEU:HD13	1.55	0.85
4:n:100:GLY:C	5:p:76:A:H3'	2.02	0.85
6:a:19:G:H1'	6:a:57:G:N2	1.92	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:12:ALA:HB1	4:n:52:SER:HA	1.59	0.84
1:y:415:ASP:CB	4:n:39:HIS:HD2	1.90	0.84
1:y:12:ALA:HB2	4:n:52:SER:O	1.76	0.84
4:n:72:ALA:C	4:n:76:VAL:HG23	2.03	0.84
4:n:100:GLY:C	5:p:76:A:C3'	2.50	0.84
1:y:146:GLN:HA	4:n:30:LEU:HD13	1.56	0.84
4:n:72:ALA:CB	4:n:76:VAL:CG2	2.56	0.84
1:y:253:GLN:CB	11:1:91:A:H61	1.87	0.83
4:n:11:LEU:HD13	4:n:36:PHE:CE1	2.11	0.83
4:n:62:MET:HG3	9:U:51:LEU:HA	1.59	0.83
3:G:41:THR:CG2	4:n:40:GLN:NE2	2.41	0.83
1:y:250:LYS:NZ	11:1:63:A:H4'	1.94	0.82
1:y:250:LYS:HZ1	11:1:63:A:H4'	1.41	0.82
2:E:81:LYS:HD3	8:T:93:LEU:CD1	2.05	0.82
4:n:85:PHE:HD1	4:n:87:THR:HG23	0.94	0.82
4:n:56:LEU:HD23	4:n:56:LEU:N	1.93	0.82
1:y:415:ASP:CG	4:n:41:ARG:HB3	2.05	0.82
1:y:139:LEU:CD2	4:n:33:GLN:HG2	2.11	0.81
6:a:10:G:H3'	6:a:11:C:H5	1.43	0.81
5:p:47:U:O4	6:a:17:C:P	2.39	0.81
4:n:73:VAL:HG22	4:n:77:ALA:CB	2.10	0.81
1:y:415:ASP:CA	4:n:41:ARG:CB	2.55	0.80
1:y:139:LEU:HD21	4:n:33:GLN:CG	2.10	0.80
1:y:293:TRP:HE1	4:n:22:TYR:HD2	1.09	0.80
1:y:242:ARG:HH22	10:Y:36:GLN:HB3	1.45	0.80
1:y:57:ARG:HG2	4:n:27:SER:OG	1.81	0.80
1:y:293:TRP:CZ2	4:n:22:TYR:CG	2.69	0.80
4:n:60:VAL:O	4:n:61:LYS:HB2	1.82	0.79
1:y:415:ASP:OD2	4:n:41:ARG:HB3	1.82	0.79
4:n:28:GLY:O	4:n:29:GLU:HB2	1.83	0.79
1:y:415:ASP:CB	4:n:39:HIS:CD2	2.66	0.79
4:n:85:PHE:CD1	4:n:87:THR:HG22	2.16	0.79
6:a:74:C:C2'	6:a:75:C:H5'	2.13	0.78
2:E:78:GLU:HA	8:T:93:LEU:HD13	1.64	0.78
1:y:83:MET:CB	4:n:36:PHE:HB2	2.13	0.78
1:y:9:PHE:HA	4:n:52:SER:HB2	1.65	0.78
6:a:2:C:H2'	6:a:3:C:C6	2.18	0.78
4:n:46:ASP:CG	9:U:52:ASN:HD21	1.92	0.78
1:y:86:ILE:HG13	4:n:36:PHE:CD2	2.19	0.77
4:n:72:ALA:HB1	4:n:76:VAL:CG2	2.13	0.77
4:n:42:SER:O	4:n:43:ILE:HD12	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:n:64:LYS:HG2	4:n:65:TYR:H	1.50	0.76
4:n:11:LEU:HD12	4:n:36:PHE:HE1	1.47	0.76
4:n:73:VAL:HG13	4:n:74:ALA:CA	2.13	0.76
1:y:12:ALA:HB3	4:n:52:SER:HA	1.68	0.75
1:y:64:PHE:HD2	4:n:21:GLN:HG2	1.50	0.75
6:a:60:U:H5'	6:a:61:C:OP2	1.86	0.75
1:y:188:SER:HB3	4:n:39:HIS:CG	2.21	0.75
1:y:356:ILE:HA	8:T:18:GLU:CB	2.08	0.75
1:y:52:LEU:HB3	4:n:29:GLU:CG	2.11	0.75
1:y:242:ARG:NH2	10:Y:36:GLN:CB	2.51	0.74
4:n:52:SER:OG	4:n:55:SER:CB	2.35	0.74
3:G:41:THR:HG21	4:n:40:GLN:NE2	2.01	0.74
4:n:85:PHE:HE1	4:n:87:THR:HG21	1.53	0.74
1:y:147:GLY:H	4:n:30:LEU:CD1	1.99	0.74
1:y:279:PHE:CD2	4:n:13:LEU:HB2	2.23	0.74
4:n:28:GLY:O	4:n:29:GLU:CB	2.36	0.73
1:y:257:VAL:CG2	11:1:93:G:N3	2.51	0.73
2:E:81:LYS:CD	8:T:93:LEU:CG	2.67	0.73
4:n:42:SER:O	4:n:43:ILE:CB	2.35	0.73
4:n:42:SER:O	4:n:43:ILE:CG1	2.35	0.73
3:G:34:PHE:CD1	3:G:36:ALA:HB3	2.22	0.73
4:n:62:MET:CG	9:U:51:LEU:CD2	2.66	0.73
1:y:86:ILE:HG21	4:n:36:PHE:CE2	2.23	0.73
1:y:253:GLN:CG	11:1:91:A:H61	2.01	0.73
1:y:257:VAL:HG23	11:1:93:G:C2	2.24	0.72
3:G:41:THR:HG22	4:n:40:GLN:NE2	2.03	0.72
4:n:62:MET:HG3	9:U:51:LEU:CD2	2.17	0.72
4:n:61:LYS:O	4:n:62:MET:CB	2.36	0.72
4:n:61:LYS:O	9:U:51:LEU:CD2	2.38	0.72
1:y:202:ALA:HB1	1:y:401:PHE:CZ	2.24	0.72
4:n:23:GLU:O	4:n:24:ASP:CB	2.36	0.71
1:y:188:SER:HB3	4:n:39:HIS:ND1	2.05	0.71
1:y:256:ARG:C	11:1:93:G:H1'	2.15	0.71
4:n:41:ARG:O	4:n:41:ARG:HG3	1.78	0.71
1:y:16:LEU:CD2	4:n:53:TYR:HE2	2.04	0.71
1:y:253:GLN:CG	11:1:91:A:N6	2.54	0.71
1:y:242:ARG:HH22	10:Y:36:GLN:CB	2.05	0.70
1:y:16:LEU:CD1	4:n:53:TYR:OH	2.34	0.70
1:y:185:ASN:CB	4:n:39:HIS:CE1	2.61	0.70
1:y:242:ARG:NH2	10:Y:36:GLN:HB3	2.07	0.70
1:y:56:GLN:O	1:y:61:ILE:CG2	2.40	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:418:ALA:HB1	4:n:41:ARG:O	1.89	0.70
4:n:61:LYS:C	4:n:62:MET:HG2	2.15	0.69
1:y:83:MET:HB2	4:n:36:PHE:CB	2.20	0.69
4:n:71:LEU:O	4:n:72:ALA:C	2.33	0.69
6:a:74:C:H1'	6:a:75:C:H5'	1.74	0.69
4:n:32:ARG:HG3	4:n:34:HIS:H	1.57	0.69
1:y:147:GLY:H	4:n:30:LEU:HD13	1.57	0.69
1:y:415:ASP:CB	4:n:41:ARG:HB3	2.23	0.69
6:a:9:A:H2	6:a:11:C:H41	1.41	0.69
4:n:52:SER:CB	4:n:55:SER:HB3	2.23	0.68
2:E:81:LYS:HD3	8:T:93:LEU:CG	2.22	0.68
4:n:73:VAL:CG1	4:n:74:ALA:HA	2.22	0.68
6:a:9:A:O2'	6:a:10:G:OP1	2.12	0.68
1:y:252:GLN:NE2	8:T:70:HIS:CG	2.59	0.67
4:n:52:SER:C	4:n:54:HIS:H	2.00	0.67
1:y:345:ASN:ND2	4:n:2:LYS:NZ	2.43	0.67
1:y:361:GLN:HG3	8:T:19:LYS:HD3	1.76	0.67
1:y:257:VAL:CB	11:1:93:G:N3	2.57	0.67
1:y:375:LEU:HB3	2:E:79:VAL:HG11	1.77	0.67
4:n:73:VAL:HG13	12:2:1322:A:O2'	1.95	0.67
4:n:41:ARG:CZ	4:n:43:ILE:HD11	2.25	0.67
4:n:42:SER:O	4:n:43:ILE:HB	1.93	0.66
1:y:86:ILE:HG21	4:n:36:PHE:CZ	2.31	0.66
6:a:10:G:H3'	6:a:11:C:C5	2.27	0.66
1:y:52:LEU:CD2	4:n:29:GLU:HB3	2.25	0.66
1:y:64:PHE:HE1	4:n:32:ARG:HH21	1.41	0.66
4:n:43:ILE:O	4:n:45:GLY:N	2.29	0.66
4:n:59:GLY:O	4:n:60:VAL:CB	2.43	0.65
1:y:419:GLN:NE2	4:n:3:LYS:NZ	2.41	0.65
1:y:188:SER:HB3	4:n:39:HIS:CE1	2.31	0.65
4:n:11:LEU:CD1	4:n:36:PHE:CD1	2.80	0.65
1:y:52:LEU:HB3	4:n:29:GLU:OE1	1.96	0.65
4:n:11:LEU:HD12	4:n:36:PHE:CD1	2.32	0.65
1:y:12:ALA:CB	4:n:52:SER:O	2.45	0.65
1:y:52:LEU:HB3	4:n:29:GLU:CB	1.98	0.65
1:y:8:ASP:C	4:n:55:SER:HB2	2.22	0.64
4:n:42:SER:O	4:n:43:ILE:CD1	2.45	0.64
4:n:23:GLU:HB2	4:n:31:GLU:HB3	1.80	0.64
4:n:99:ALA:C	4:n:100:GLY:CA	2.69	0.64
4:n:32:ARG:NH1	4:n:34:HIS:HA	2.09	0.64
4:n:51:HIS:O	4:n:52:SER:CB	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:86:ILE:HD12	4:n:36:PHE:HE2	1.62	0.64
4:n:60:VAL:O	4:n:61:LYS:CB	2.45	0.64
6:a:74:C:O2'	6:a:75:C:P	2.56	0.64
4:n:43:ILE:O	4:n:44:SER:C	2.40	0.63
4:n:32:ARG:NH1	4:n:34:HIS:CB	2.61	0.63
6:a:74:C:O2'	6:a:75:C:OP2	2.16	0.63
4:n:51:HIS:CD2	4:n:52:SER:H	2.16	0.63
6:a:23:A:H2'	6:a:24:G:O4'	1.99	0.63
4:n:62:MET:CB	9:U:51:LEU:HD23	2.27	0.63
6:a:9:A:H2	6:a:11:C:N4	1.96	0.63
4:n:73:VAL:HA	4:n:74:ALA:C	2.24	0.63
1:y:202:ALA:HB1	1:y:401:PHE:CE2	2.34	0.63
4:n:42:SER:OG	4:n:43:ILE:N	2.30	0.62
4:n:49:SER:C	4:n:51:HIS:H	2.06	0.62
4:n:52:SER:O	4:n:54:HIS:N	2.31	0.62
6:a:75:C:H3'	6:a:75:C:H6	1.63	0.62
1:y:52:LEU:HB2	4:n:29:GLU:HG3	1.64	0.62
4:n:14:ALA:CB	4:n:18:SER:H	2.12	0.62
6:a:19:G:H1'	6:a:57:G:C2	2.35	0.62
1:y:31:ILE:HD12	2:E:114:ILE:HB	1.81	0.62
1:y:86:ILE:HG13	4:n:36:PHE:HD2	1.64	0.62
1:y:257:VAL:HA	11:1:92:U:N3	2.10	0.61
1:y:142:MET:HB2	4:n:31:GLU:OE2	2.00	0.61
4:n:32:ARG:HG3	4:n:33:GLN:H	0.54	0.61
6:a:74:C:C1'	6:a:75:C:H5'	2.30	0.61
1:y:415:ASP:CB	4:n:41:ARG:CB	2.78	0.61
6:a:74:C:O2'	6:a:75:C:C6	2.52	0.61
1:y:64:PHE:CE1	4:n:32:ARG:NH2	2.68	0.61
1:y:415:ASP:C	4:n:39:HIS:CD2	2.79	0.61
4:n:32:ARG:C	4:n:33:GLN:HG2	2.22	0.61
1:y:279:PHE:HB2	4:n:13:LEU:HD22	1.82	0.61
4:n:64:LYS:CG	4:n:65:TYR:N	2.59	0.61
4:n:14:ALA:HB1	4:n:18:SER:H	1.65	0.60
4:n:47:GLY:O	4:n:48:ASP:CB	2.49	0.60
6:a:19:G:C1'	6:a:57:G:N2	2.64	0.60
1:y:12:ALA:CB	4:n:52:SER:C	2.74	0.60
6:a:5:G:H2'	6:a:6:G:H8	1.65	0.60
1:y:83:MET:HA	4:n:36:PHE:HB3	1.82	0.60
1:y:356:ILE:CA	8:T:18:GLU:HB3	2.25	0.60
6:a:2:C:H2'	6:a:3:C:H6	1.63	0.60
4:n:32:ARG:NH1	4:n:34:HIS:CG	2.69	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:a:5:G:O2'	6:a:6:G:H5'	2.02	0.59
4:n:64:LYS:CG	4:n:65:TYR:H	2.15	0.59
1:y:365:TYR:HE1	8:T:26:LYS:HZ3	1.48	0.59
3:G:36:ALA:HB1	3:G:40:ALA:HB3	1.85	0.59
4:n:99:ALA:N	4:n:100:GLY:N	2.50	0.59
1:y:275:ILE:CD1	4:n:6:LEU:CD1	2.68	0.59
4:n:39:HIS:O	4:n:40:GLN:HG2	2.02	0.59
1:y:12:ALA:HB1	4:n:52:SER:CA	2.30	0.59
4:n:60:VAL:O	4:n:60:VAL:HG13	2.03	0.59
1:y:293:TRP:NE1	4:n:22:TYR:CG	2.68	0.58
4:n:51:HIS:CD2	4:n:52:SER:N	2.71	0.58
4:n:82:LEU:HD21	4:n:84:LEU:HG	1.85	0.58
4:n:36:PHE:CD2	4:n:36:PHE:O	2.56	0.58
1:y:419:GLN:NE2	4:n:3:LYS:CE	2.65	0.58
4:n:72:ALA:HB1	4:n:76:VAL:HG21	1.75	0.58
1:y:365:TYR:CZ	8:T:22:THR:CB	2.86	0.58
2:E:81:LYS:HD2	8:T:93:LEU:HD12	0.59	0.58
1:y:7:LEU:H	1:y:7:LEU:HD23	1.69	0.58
4:n:13:LEU:HD12	4:n:13:LEU:O	2.03	0.58
4:n:73:VAL:CG1	12:2:1322:A:H1'	2.34	0.58
1:y:83:MET:CA	4:n:36:PHE:HB3	2.33	0.58
1:y:83:MET:HA	4:n:36:PHE:CB	2.35	0.57
6:a:11:C:H2'	6:a:12:U:C6	2.39	0.57
4:n:32:ARG:HH11	4:n:34:HIS:CA	2.12	0.57
6:a:19:G:HO2'	6:a:20:U:P	2.27	0.57
1:y:293:TRP:HZ2	4:n:22:TYR:CE2	2.21	0.57
4:n:71:LEU:O	4:n:73:VAL:O	2.23	0.57
4:n:23:GLU:N	4:n:31:GLU:HB3	2.20	0.56
1:y:31:ILE:CD1	2:E:114:ILE:HB	2.35	0.56
1:y:12:ALA:HB2	4:n:52:SER:C	2.29	0.56
1:y:279:PHE:CG	4:n:13:LEU:HB2	2.41	0.56
1:y:293:TRP:NE1	4:n:22:TYR:HB2	2.18	0.56
4:n:26:SER:O	4:n:27:SER:HB3	2.06	0.56
1:y:419:GLN:HE22	4:n:3:LYS:HZ2	1.49	0.56
1:y:250:LYS:NZ	11:1:63:A:C4'	2.65	0.56
1:y:139:LEU:HD22	4:n:32:ARG:O	2.05	0.56
4:n:73:VAL:HG11	12:2:1322:A:C2'	2.35	0.56
1:y:196:VAL:HG21	2:E:111:LEU:HD13	1.87	0.56
1:y:416:PHE:N	4:n:39:HIS:CD2	2.74	0.56
4:n:32:ARG:NH1	4:n:34:HIS:CA	2.69	0.56
4:n:73:VAL:HG11	12:2:1322:A:H1'	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:n:32:ARG:HG3	4:n:34:HIS:N	2.20	0.55
6:a:42:C:O2'	6:a:43:C:H5'	2.06	0.55
1:y:117:SER:HB2	3:G:36:ALA:C	2.31	0.55
1:y:275:ILE:HD13	4:n:6:LEU:HD11	1.80	0.55
1:y:356:ILE:CA	8:T:18:GLU:CB	2.73	0.55
6:a:56:C:H2'	6:a:57:G:H8	1.71	0.55
1:y:86:ILE:HD12	4:n:36:PHE:CE2	2.40	0.55
3:G:29:ASP:O	3:G:33:SER:HB2	2.06	0.55
4:n:72:ALA:C	4:n:76:VAL:CG2	2.72	0.55
5:p:4:G:H2'	5:p:5:G:H5''	1.89	0.55
4:n:60:VAL:O	4:n:60:VAL:CG1	2.55	0.55
1:y:415:ASP:C	4:n:39:HIS:HD2	2.15	0.55
4:n:99:ALA:CA	4:n:100:GLY:N	2.67	0.55
6:a:51:U:H2'	6:a:52:G:C8	2.40	0.55
6:a:19:G:N2	6:a:56:C:N3	2.55	0.55
1:y:279:PHE:CB	4:n:13:LEU:HD13	2.37	0.54
5:p:47:U:O4	6:a:17:C:OP2	2.24	0.54
6:a:8:U:OP2	6:a:8:U:H6	1.89	0.54
6:a:11:C:H2'	6:a:12:U:H6	1.72	0.54
6:a:58:A:H4'	6:a:59:U:OP1	2.07	0.54
6:a:61:C:O2'	6:a:62:C:H5'	2.06	0.54
1:y:280:ALA:HA	1:y:332:TYR:CE1	2.43	0.54
1:y:415:ASP:HB3	4:n:39:HIS:CD2	2.41	0.54
1:y:293:TRP:CG	4:n:22:TYR:HB2	2.40	0.54
4:n:46:ASP:OD2	9:U:52:ASN:ND2	2.41	0.54
1:y:230:VAL:HG11	1:y:406:LEU:HD22	1.90	0.54
1:y:254:GLY:N	11:1:91:A:C5	2.75	0.54
1:y:357:ARG:NH2	12:2:1337:G:O2'	2.40	0.54
4:n:37:ALA:O	4:n:38:LEU:CB	2.47	0.54
4:n:55:SER:C	4:n:56:LEU:HD22	2.29	0.54
4:n:67:GLN:O	4:n:68:GLU:C	2.50	0.54
4:n:63:THR:CG2	4:n:64:LYS:N	2.42	0.54
4:n:61:LYS:O	9:U:51:LEU:HD22	2.08	0.53
6:a:51:U:H2'	6:a:52:G:H8	1.73	0.53
1:y:252:GLN:NE2	8:T:70:HIS:CD2	2.76	0.53
4:n:76:VAL:HG12	4:n:76:VAL:O	2.08	0.53
4:n:71:LEU:O	4:n:72:ALA:O	2.26	0.53
1:y:41:ILE:HG22	1:y:43:GLY:H	1.73	0.53
1:y:253:GLN:HG3	11:1:91:A:H61	1.70	0.53
1:y:274:VAL:HG11	1:y:410:VAL:CG1	2.38	0.53
6:a:25:C:H5'	6:a:26:A:OP2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:a:22:G:N7	6:a:46:G:N2	2.57	0.53
1:y:37:SER:HA	1:y:77:ILE:CG2	2.39	0.53
1:y:52:LEU:HB3	4:n:29:GLU:CD	2.32	0.53
1:y:52:LEU:HD22	4:n:29:GLU:HB3	1.90	0.53
1:y:12:ALA:HB2	4:n:52:SER:CA	2.35	0.53
1:y:40:PRO:O	3:G:68:LEU:HD22	2.08	0.53
1:y:254:GLY:HA2	11:1:91:A:C1'	2.35	0.53
14:4:2103:C:C5	14:4:2104:C:C6	2.97	0.53
1:y:418:ALA:HB1	4:n:42:SER:OG	2.09	0.52
1:y:16:LEU:HD22	4:n:53:TYR:HE2	1.74	0.52
1:y:415:ASP:CA	4:n:41:ARG:HB3	2.39	0.52
4:n:32:ARG:O	4:n:33:GLN:NE2	2.42	0.52
6:a:69:G:C2'	6:a:70:G:H5''	2.29	0.52
1:y:345:ASN:ND2	4:n:2:LYS:HZ2	2.07	0.52
1:y:57:ARG:H	4:n:27:SER:HB3	1.73	0.52
4:n:32:ARG:O	4:n:33:GLN:CD	2.53	0.52
4:n:82:LEU:HD21	4:n:84:LEU:CD1	2.40	0.52
1:y:333:THR:HB	1:y:374:THR:HB	1.92	0.52
6:a:46:G:H5''	6:a:47:U:OP2	2.10	0.52
1:y:117:SER:HB3	3:G:36:ALA:HA	1.92	0.52
1:y:290:ILE:HD13	1:y:293:TRP:CH2	2.45	0.52
1:y:345:ASN:ND2	4:n:2:LYS:HZ1	2.08	0.52
1:y:361:GLN:HG3	8:T:19:LYS:CD	2.40	0.52
6:a:24:G:N3	6:a:24:G:H2'	2.25	0.52
1:y:83:MET:CA	4:n:36:PHE:CB	2.88	0.51
4:n:23:GLU:CB	4:n:31:GLU:HB3	2.40	0.51
4:n:91:ILE:HG22	4:n:91:ILE:O	2.10	0.51
4:n:34:HIS:HE2	4:n:37:ALA:H	1.56	0.51
6:a:55:U:H2'	6:a:57:G:OP2	2.10	0.51
1:y:176:GLU:CB	3:G:37:GLY:HA2	2.41	0.51
4:n:43:ILE:O	4:n:45:GLY:CA	2.59	0.51
4:n:98:ARG:O	4:n:98:ARG:HG2	2.10	0.51
6:a:19:G:O2'	6:a:20:U:P	2.68	0.51
6:a:23:A:H2'	6:a:24:G:C1'	2.40	0.51
1:y:16:LEU:HD22	4:n:53:TYR:CE2	2.43	0.51
6:a:33:U:O4'	6:a:37:MIA:H161	2.10	0.51
1:y:9:PHE:HB2	4:n:55:SER:OG	2.11	0.51
1:y:365:TYR:OH	8:T:22:THR:CB	2.55	0.51
6:a:11:C:O2'	6:a:12:U:H5'	2.10	0.51
6:a:37:MIA:H3'	6:a:38:A:H8	1.76	0.51
1:y:146:GLN:HA	4:n:30:LEU:CD1	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:a:11:C:H6	6:a:11:C:O5'	1.93	0.51
1:y:415:ASP:HB3	4:n:41:ARG:CA	2.42	0.50
1:y:9:PHE:N	4:n:55:SER:CB	2.74	0.50
1:y:139:LEU:CD2	4:n:33:GLN:CG	2.82	0.50
3:G:36:ALA:HB1	3:G:40:ALA:CB	2.42	0.50
4:n:62:MET:HB2	9:U:51:LEU:HD23	1.92	0.50
1:y:357:ARG:HH11	12:2:1336:A:H2	1.59	0.50
4:n:34:HIS:CD2	4:n:35:THR:O	2.65	0.50
1:y:361:GLN:CG	8:T:19:LYS:HD3	2.41	0.50
1:y:199:LEU:HG	1:y:203:ILE:HG12	1.92	0.50
1:y:293:TRP:NE1	4:n:22:TYR:CB	2.73	0.50
1:y:254:GLY:HA2	11:1:91:A:C5	2.46	0.50
4:n:41:ARG:O	4:n:41:ARG:CG	2.28	0.50
4:n:65:TYR:O	4:n:65:TYR:CD1	2.66	0.49
1:y:293:TRP:CD1	4:n:22:TYR:HB2	2.47	0.49
1:y:37:SER:HA	1:y:77:ILE:HG23	1.92	0.49
1:y:9:PHE:N	4:n:55:SER:HB2	2.28	0.49
1:y:31:ILE:HD12	2:E:114:ILE:CB	2.43	0.49
6:a:57:G:H2'	6:a:58:A:H5''	1.94	0.49
4:n:42:SER:C	4:n:43:ILE:HG13	2.38	0.49
4:n:29:GLU:O	4:n:30:LEU:O	2.30	0.49
14:4:2103:C:C5	14:4:2104:C:C5	3.01	0.49
1:y:139:LEU:CD2	4:n:32:ARG:O	2.61	0.48
6:a:5:G:H2'	6:a:6:G:C8	2.46	0.48
6:a:7:A:C5'	6:a:8:U:OP2	2.53	0.48
6:a:19:G:O2'	6:a:20:U:OP2	2.29	0.48
6:a:75:C:H3'	6:a:75:C:C6	2.46	0.48
1:y:180:GLU:HB3	3:G:46:SER:C	2.38	0.48
4:n:55:SER:O	4:n:56:LEU:HD22	2.13	0.48
6:a:42:C:H2'	6:a:43:C:C6	2.48	0.48
14:4:2111:U:H3'	14:4:2112:G:H5'	1.94	0.48
1:y:30:LEU:HB3	2:E:111:LEU:HD11	1.94	0.48
4:n:28:GLY:O	4:n:29:GLU:HG2	2.13	0.48
4:n:67:GLN:O	4:n:68:GLU:O	2.30	0.48
1:y:257:VAL:HG21	11:1:93:G:H21	1.67	0.48
6:a:23:A:H2'	6:a:24:G:C8	2.48	0.48
4:n:49:SER:O	4:n:51:HIS:N	2.46	0.48
4:n:14:ALA:HB1	4:n:18:SER:N	2.29	0.48
7:5:172:HIS:CD2	14:4:2123:G:H21	2.32	0.48
1:y:69:GLY:HA2	1:y:408:ILE:HG23	1.96	0.48
4:n:28:GLY:O	4:n:29:GLU:CG	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:n:73:VAL:HG11	12:2:1322:A:C1'	2.43	0.48
1:y:57:ARG:HH11	1:y:61:ILE:HA	1.78	0.47
7:5:53:ARG:HB3	7:5:167:LYS:HA	1.95	0.47
4:n:34:HIS:CG	4:n:35:THR:N	2.83	0.47
4:n:75:ALA:C	4:n:77:ALA:H	2.22	0.47
6:a:21:A:N6	6:a:46:G:C4	2.82	0.47
11:1:82:U:H3	11:1:104:A:H61	1.62	0.47
6:a:9:A:C2	6:a:11:C:N4	2.80	0.47
4:n:26:SER:O	4:n:27:SER:CB	2.63	0.47
1:y:12:ALA:HB1	4:n:52:SER:C	2.39	0.47
1:y:242:ARG:NH2	10:Y:36:GLN:HA	2.30	0.47
4:n:41:ARG:NE	4:n:43:ILE:HD11	2.30	0.47
6:a:34:G:O2'	6:a:35:A:H5'	2.15	0.47
1:y:83:MET:N	4:n:36:PHE:HB3	2.30	0.47
1:y:185:ASN:HB2	4:n:39:HIS:HE1	1.73	0.47
1:y:256:ARG:O	11:1:92:U:O2	0.53	0.47
4:n:73:VAL:CG1	12:2:1322:A:C1'	2.94	0.46
14:4:2091:C:H3'	14:4:2092:U:H5''	1.97	0.46
1:y:147:GLY:H	4:n:30:LEU:HD11	1.79	0.46
2:E:84:TRP:HB2	2:E:85:PRO:HD3	1.97	0.46
6:a:42:C:H2'	6:a:43:C:H6	1.81	0.46
1:y:64:PHE:CE2	4:n:19:CYS:HB3	2.51	0.46
4:n:42:SER:C	4:n:43:ILE:CG1	2.88	0.46
4:n:73:VAL:CG1	4:n:74:ALA:N	2.79	0.46
6:a:8:U:O2'	6:a:9:A:C5'	2.63	0.46
4:n:52:SER:C	4:n:54:HIS:N	2.66	0.46
4:n:32:ARG:HD2	4:n:34:HIS:HA	1.98	0.46
4:n:49:SER:C	4:n:51:HIS:N	2.71	0.46
6:a:16:U:H2'	6:a:18:G:OP2	2.15	0.46
14:4:2110:G:H3'	14:4:2111:U:H5'	1.98	0.46
1:y:202:ALA:HB1	1:y:401:PHE:HZ	1.76	0.46
6:a:22:G:O2'	6:a:23:A:H5'	2.15	0.46
11:1:63:A:H2'	11:1:64:A:C8	2.51	0.46
1:y:117:SER:CB	3:G:36:ALA:HA	2.46	0.46
4:n:52:SER:OG	4:n:55:SER:N	2.49	0.46
2:E:107:ILE:O	2:E:111:LEU:HD12	2.16	0.45
6:a:75:C:C6	6:a:75:C:C3'	2.99	0.45
1:y:176:GLU:HB2	3:G:37:GLY:HA2	1.98	0.45
1:y:330:PHE:CD2	1:y:375:LEU:HD12	2.52	0.45
7:5:212:VAL:O	7:5:223:ALA:HB1	2.16	0.45
1:y:64:PHE:CZ	4:n:32:ARG:NH2	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:290:ILE:HD13	1:y:293:TRP:CZ2	2.52	0.45
4:n:32:ARG:C	4:n:33:GLN:CG	2.87	0.45
4:n:23:GLU:HG3	4:n:29:GLU:C	2.33	0.45
6:a:66:U:H2'	6:a:67:C:C6	2.51	0.45
1:y:145:MET:SD	4:n:30:LEU:HD23	2.49	0.45
3:G:37:GLY:O	3:G:38:ALA:HB2	2.17	0.45
1:y:86:ILE:CG1	4:n:36:PHE:CD2	2.98	0.44
1:y:415:ASP:HB3	4:n:41:ARG:HA	1.98	0.44
4:n:74:ALA:O	4:n:75:ALA:C	2.60	0.44
6:a:39:U:H2'	6:a:40:C:H6	1.82	0.44
1:y:242:ARG:NH2	10:Y:36:GLN:CA	2.80	0.44
6:a:21:A:N7	6:a:46:G:C6	2.85	0.44
1:y:8:ASP:CB	4:n:54:HIS:O	2.54	0.44
1:y:35:ILE:HG22	2:E:115:LEU:HA	2.00	0.44
3:G:68:LEU:HG	3:G:69:VAL:N	2.33	0.44
5:p:12:U:H3	5:p:23:A:H61	1.65	0.44
3:G:32:ALA:HB3	3:G:53:THR:HG21	1.99	0.44
4:n:89:VAL:HG13	4:n:89:VAL:O	2.18	0.44
1:y:188:SER:HB3	4:n:39:HIS:CD2	2.53	0.44
4:n:73:VAL:CG1	4:n:74:ALA:CA	2.90	0.44
6:a:17:C:H5'	6:a:18:G:OP2	2.18	0.44
1:y:405:SER:O	1:y:408:ILE:HB	2.17	0.44
1:y:416:PHE:N	4:n:39:HIS:HD2	2.15	0.44
4:n:91:ILE:O	4:n:92:SER:C	2.61	0.44
4:n:72:ALA:HB1	4:n:76:VAL:CG1	2.46	0.43
7:5:156:ALA:HA	7:5:160:GLN:HB3	2.00	0.43
1:y:254:GLY:CA	11:1:91:A:C5	3.00	0.43
1:y:274:VAL:HG11	1:y:410:VAL:HG12	2.00	0.43
1:y:172:MET:CB	3:G:38:ALA:HA	2.48	0.43
1:y:357:ARG:NH1	12:2:1337:G:H1'	2.33	0.43
4:n:11:LEU:CD1	4:n:36:PHE:HE1	2.10	0.43
4:n:32:ARG:NH1	4:n:34:HIS:HB2	2.32	0.43
1:y:83:MET:CB	4:n:36:PHE:CB	2.87	0.43
1:y:146:GLN:N	4:n:30:LEU:HD22	2.34	0.43
4:n:47:GLY:O	4:n:48:ASP:HB3	2.18	0.43
4:n:74:ALA:O	4:n:77:ALA:HB3	2.19	0.43
4:n:74:ALA:O	4:n:77:ALA:N	2.51	0.43
5:p:74:C:C5	5:p:75:C:C2	3.07	0.43
4:n:72:ALA:O	4:n:73:VAL:C	2.62	0.43
6:a:44:G:H2'	6:a:45:U:C6	2.54	0.43
1:y:86:ILE:CG1	4:n:36:PHE:CE2	3.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:5:79:THR:HB	7:5:81:GLY:H	1.84	0.43
1:y:113:ARG:C	3:G:36:ALA:HB2	2.43	0.43
1:y:196:VAL:HG22	2:E:108:LEU:HD23	2.00	0.43
7:5:14:LYS:HB2	7:5:17:ALA:HB2	2.00	0.43
4:n:69:GLN:OE1	4:n:71:LEU:CD1	2.67	0.43
1:y:64:PHE:CD2	4:n:21:GLN:HG2	2.40	0.42
1:y:135:ILE:HG23	4:n:33:GLN:HG3	2.00	0.42
1:y:139:LEU:HD21	4:n:33:GLN:HG3	1.97	0.42
1:y:358:PRO:HG2	12:2:1317:G:H4'	2.01	0.42
1:y:52:LEU:HG	1:y:53:LEU:H	1.84	0.42
1:y:57:ARG:HA	4:n:26:SER:O	2.19	0.42
1:y:86:ILE:CD1	4:n:36:PHE:HE2	2.31	0.42
4:n:82:LEU:HD21	4:n:84:LEU:CG	2.48	0.42
5:p:9:A:H61	5:p:22:G:H3'	1.84	0.42
1:y:26:VAL:O	1:y:30:LEU:HD12	2.19	0.42
1:y:52:LEU:HG	1:y:53:LEU:N	2.35	0.42
1:y:419:GLN:HE22	4:n:3:LYS:CD	2.33	0.42
4:n:23:GLU:HG2	4:n:29:GLU:O	2.10	0.42
1:y:38:PHE:O	1:y:47:ALA:HB2	2.19	0.42
1:y:39:ILE:HG22	3:G:68:LEU:HD21	2.01	0.42
4:n:32:ARG:CG	4:n:34:HIS:H	2.30	0.42
4:n:36:PHE:O	4:n:36:PHE:CG	2.72	0.42
4:n:62:MET:HG2	9:U:51:LEU:CD2	2.47	0.42
6:a:58:A:O2'	6:a:59:U:P	2.78	0.42
1:y:250:LYS:HB2	12:2:1336:A:O5'	2.19	0.42
4:n:29:GLU:O	4:n:30:LEU:C	2.63	0.41
6:a:18:G:O2'	6:a:19:G:P	2.77	0.41
7:5:12:ARG:HE	14:4:2107:G:H4'	1.84	0.41
1:y:146:GLN:HA	4:n:30:LEU:HD22	2.02	0.41
1:y:145:MET:C	4:n:30:LEU:CD2	2.80	0.41
4:n:61:LYS:HD2	4:n:61:LYS:HA	1.35	0.41
1:y:31:ILE:HD13	1:y:31:ILE:HA	1.83	0.41
1:y:66:MET:HA	1:y:408:ILE:CG1	2.50	0.41
1:y:415:ASP:CG	4:n:40:GLN:O	2.64	0.41
1:y:150:ILE:HD12	1:y:150:ILE:HA	1.92	0.41
4:n:69:GLN:OE1	4:n:71:LEU:HD13	2.20	0.41
6:a:16:U:H2'	6:a:17:C:H5'	2.03	0.41
6:a:67:C:H2'	6:a:68:C:C6	2.55	0.41
4:n:11:LEU:O	4:n:14:ALA:HB3	2.21	0.41
5:p:47:U:C4	5:p:50:C:H5''	2.55	0.41
7:5:76:ALA:HB1	7:5:103:GLN:NE2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:y:371:THR:O	1:y:375:LEU:HD22	2.21	0.41
1:y:49:LEU:HA	1:y:52:LEU:CD2	2.51	0.40
1:y:375:LEU:HB3	2:E:79:VAL:CG1	2.49	0.40
1:y:64:PHE:HE1	4:n:32:ARG:NH2	2.09	0.40
4:n:72:ALA:CB	4:n:76:VAL:HB	2.36	0.40
14:4:2194:U:H2'	14:4:2195:U:C6	2.57	0.40
1:y:419:GLN:NE2	4:n:3:LYS:HZ3	2.15	0.40
1:y:419:GLN:CD	4:n:3:LYS:HZ3	2.28	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	y	435/437 (100%)	392 (90%)	18 (4%)	25 (6%)	1	14
2	E	54/56 (96%)	49 (91%)	4 (7%)	1 (2%)	6	32
3	G	65/67 (97%)	57 (88%)	4 (6%)	4 (6%)	1	13
4	n	99/101 (98%)	42 (42%)	26 (26%)	31 (31%)	0	0
7	5	232/234 (99%)	198 (85%)	25 (11%)	9 (4%)	2	19
8	T	98/100 (98%)	71 (72%)	20 (20%)	7 (7%)	1	11
9	U	101/103 (98%)	84 (83%)	14 (14%)	3 (3%)	3	23
10	Y	61/63 (97%)	48 (79%)	11 (18%)	2 (3%)	3	21
All	All	1145/1161 (99%)	941 (82%)	122 (11%)	82 (7%)	2	11

All (82) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	y	45	ASP
1	y	56	GLN

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Mol	Chain	Res	Type
1	y	258	TYR
1	y	266	PRO
1	y	298	THR
1	y	315	PRO
1	y	316	LEU
1	y	396	LYS
3	G	34	PHE
3	G	38	ALA
4	n	16	SER
4	n	24	ASP
4	n	26	SER
4	n	27	SER
4	n	30	LEU
4	n	33	GLN
4	n	37	ALA
4	n	38	LEU
4	n	39	HIS
4	n	40	GLN
4	n	43	ILE
4	n	44	SER
4	n	46	ASP
4	n	48	ASP
4	n	52	SER
4	n	60	VAL
4	n	62	MET
4	n	68	GLU
4	n	71	LEU
4	n	72	ALA
7	5	18	THR
7	5	37	LYS
7	5	120	ALA
8	T	35	ALA
8	T	36	LYS
8	T	99	ALA
9	U	49	PRO
1	y	148	LEU
1	y	210	ALA
1	y	212	GLN
1	y	399	PHE
1	y	438	LEU
1	y	439	LYS
4	n	29	GLU

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Mol	Chain	Res	Type
4	n	41	ARG
4	n	42	SER
4	n	73	VAL
4	n	76	VAL
7	5	16	ASP
7	5	159	GLY
8	T	72	GLN
10	Y	2	LYS
10	Y	37	LEU
1	y	40	PRO
1	y	400	TYR
2	E	90	THR
4	n	61	LYS
7	5	87	ALA
7	5	88	LYS
7	5	90	ALA
8	T	97	GLY
1	y	185	ASN
3	G	45	SER
4	n	57	PRO
9	U	12	VAL
9	U	75	ALA
1	y	55	GLN
1	y	78	PHE
1	y	255	ARG
4	n	50	PRO
7	5	72	SER
8	T	10	VAL
1	y	256	ARG
4	n	49	SER
8	T	29	THR
3	G	44	GLY
1	y	299	GLY
4	n	28	GLY
1	y	143	PRO
4	n	56	LEU
1	y	6	GLY
1	y	240	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	y	353/353 (100%)	329 (93%)	24 (7%)	14	36
2	E	47/47 (100%)	44 (94%)	3 (6%)	16	37
3	G	46/46 (100%)	37 (80%)	9 (20%)	1	7
4	n	77/77 (100%)	59 (77%)	18 (23%)	1	5
7	5	181/181 (100%)	172 (95%)	9 (5%)	22	43
8	T	84/84 (100%)	79 (94%)	5 (6%)	17	39
9	U	84/84 (100%)	81 (96%)	3 (4%)	31	52
10	Y	55/55 (100%)	54 (98%)	1 (2%)	51	68
All	All	927/927 (100%)	855 (92%)	72 (8%)	14	32

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	y	7	LEU
1	y	31	ILE
1	y	32	VAL
1	y	39	ILE
1	y	57	ARG
1	y	60	ILE
1	y	77	ILE
1	y	113	ARG
1	y	129	ILE
1	y	152	PRO
1	y	172	MET
1	y	176	GLU
1	y	180	GLU
1	y	189	ILE
1	y	267	LEU
1	y	290	ILE
1	y	315	PRO
1	y	336	VAL
1	y	375	LEU

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Mol	Chain	Res	Type
1	y	388	PRO
1	y	396	LYS
1	y	415	ASP
1	y	416	PHE
1	y	420	VAL
2	E	77	THR
2	E	94	THR
2	E	118	LEU
3	G	14	ILE
3	G	33	SER
3	G	34	PHE
3	G	42	LEU
3	G	43	PHE
3	G	46	SER
3	G	59	LEU
3	G	65	ILE
3	G	68	LEU
4	n	12	VAL
4	n	13	LEU
4	n	30	LEU
4	n	32	ARG
4	n	38	LEU
4	n	41	ARG
4	n	42	SER
4	n	44	SER
4	n	46	ASP
4	n	52	SER
4	n	54	HIS
4	n	56	LEU
4	n	61	LYS
4	n	67	GLN
4	n	71	LEU
4	n	73	VAL
4	n	92	SER
4	n	97	ILE
7	5	3	LYS
7	5	39	VAL
7	5	73	VAL
7	5	77	VAL
7	5	85	GLU
7	5	95	VAL
7	5	121	MET

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Mol	Chain	Res	Type
7	5	144	THR
7	5	165	ASN
8	T	36	LYS
8	T	61	LEU
8	T	66	LYS
8	T	69	ARG
8	T	96	VAL
9	U	46	LYS
9	U	49	PRO
9	U	91	LYS
10	Y	27	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	y	65	ASN
1	y	118	GLN
1	y	131	GLN
1	y	209	GLN
1	y	252	GLN
1	y	270	ASN
1	y	301	ASN
1	y	338	ASN
1	y	345	ASN
1	y	361	GLN
1	y	419	GLN
2	E	88	GLN
4	n	33	GLN
4	n	39	HIS
4	n	40	GLN
7	5	58	ASN
7	5	67	HIS
7	5	103	GLN
7	5	110	ASN
7	5	203	GLN
8	T	28	ASN
8	T	70	HIS
9	U	45	GLN
9	U	52	ASN
9	U	53	GLN
9	U	65	GLN
9	U	73	ASN

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Mol	Chain	Res	Type
10	Y	39	GLN
10	Y	41	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	1	62/63 (98%)	13 (20%)	1 (1%)
12	2	35/36 (97%)	8 (22%)	1 (2%)
13	3	43/44 (97%)	7 (16%)	2 (4%)
14	4	108/109 (99%)	39 (36%)	8 (7%)
5	p	75/76 (98%)	17 (22%)	0
6	a	75/76 (98%)	28 (37%)	0
All	All	398/404 (98%)	112 (28%)	12 (3%)

All (112) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	p	2	C
5	p	4	G
5	p	5	G
5	p	7	A
5	p	8	U
5	p	17	U
5	p	18	G
5	p	22	G
5	p	37	A
5	p	44	G
5	p	46	G
5	p	49	G
5	p	60	U
5	p	61	C
5	p	69	C
5	p	74	C
5	p	75	C
6	a	8	U
6	a	9	A
6	a	10	G
6	a	11	C
6	a	16	U
6	a	17	C
6	a	18	G

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Mol	Chain	Res	Type
6	a	19	G
6	a	20	U
6	a	21	A
6	a	22	G
6	a	24	G
6	a	25	C
6	a	26	A
6	a	27	G
6	a	41	C
6	a	44	G
6	a	46	G
6	a	47	U
6	a	49	C
6	a	58	A
6	a	59	U
6	a	61	C
6	a	70	G
6	a	73	A
6	a	74	C
6	a	75	C
6	a	76	A
11	1	63	A
11	1	64	A
11	1	71	A
11	1	74	A
11	1	75	G
11	1	84	A
11	1	90	U
11	1	91	A
11	1	92	U
11	1	93	G
11	1	95	A
11	1	100	U
11	1	103	A
12	2	1312	U
12	2	1313	U
12	2	1316	U
12	2	1325	U
12	2	1326	U
12	2	1334	G
12	2	1336	A
12	2	1337	G

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Mol	Chain	Res	Type
13	3	1523	U
13	3	1524	G
13	3	1532	A
13	3	1535	A
13	3	1538	G
13	3	1540	G
13	3	1552	A
14	4	2102	G
14	4	2104	C
14	4	2111	U
14	4	2117	A
14	4	2118	U
14	4	2119	A
14	4	2120	G
14	4	2126	A
14	4	2128	G
14	4	2129	C
14	4	2131	U
14	4	2132	U
14	4	2133	G
14	4	2135	A
14	4	2136	G
14	4	2137	U
14	4	2138	G
14	4	2144	G
14	4	2145	C
14	4	2146	C
14	4	2147	A
14	4	2148	G
14	4	2149	U
14	4	2152	G
14	4	2153	C
14	4	2155	U
14	4	2158	A
14	4	2159	G
14	4	2160	C
14	4	2163	A
14	4	2164	C
14	4	2165	C
14	4	2166	U
14	4	2176	A
14	4	2179	C

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Mol	Chain	Res	Type
14	4	2181	U
14	4	2192	U
14	4	2198	A
14	4	2199	A

All (12) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
11	1	91	A
12	2	1312	U
13	3	1535	A
13	3	1551	A
14	4	2132	U
14	4	2144	G
14	4	2145	C
14	4	2147	A
14	4	2152	G
14	4	2157	G
14	4	2163	A
14	4	2172	U

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MIA	a	37	6	28,31,32	1.57	3 (10%)	38,44,47	1.99	3 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MIA	a	37	6	-	2/15/33/34	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	a	37	MIA	C13-C14	6.14	1.50	1.32
6	a	37	MIA	C2-S10	4.34	1.79	1.75
6	a	37	MIA	C12-C13	-2.50	1.35	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	a	37	MIA	C11-S10-C2	10.54	110.16	102.25
6	a	37	MIA	C12-C13-C14	-3.48	120.76	127.01
6	a	37	MIA	C16-C14-C15	2.50	120.33	114.59

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	a	37	MIA	N6-C12-C13-C14
6	a	37	MIA	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	a	37	MIA	2	0

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	3	2
4	n	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	3	1516:G	O3'	1517:G	P	1.91
1	n	99:ALA	C	100:GLY	N	1.89
1	n	22:TYR	C	23:GLU	N	1.84
1	3	1551:A	O3'	1552:A	P	1.82

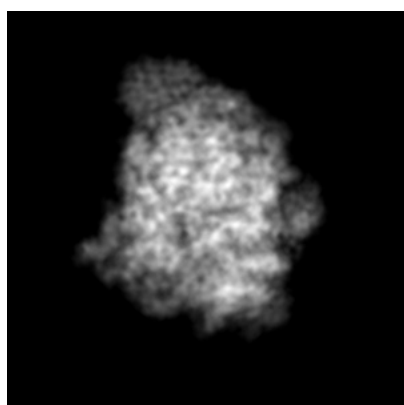
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5693. These allow visual inspection of the internal detail of the map and identification of artifacts.

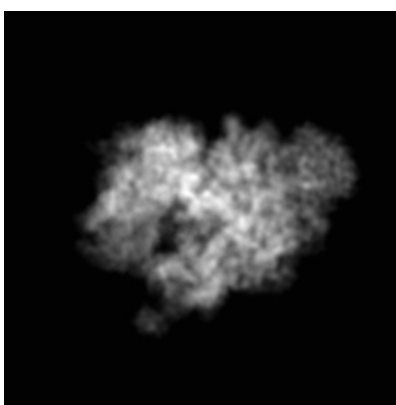
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

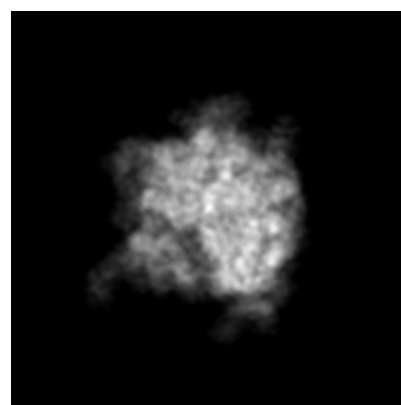
6.1.1 Primary map



X



Y

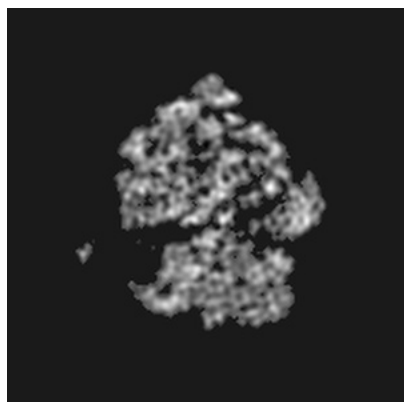


Z

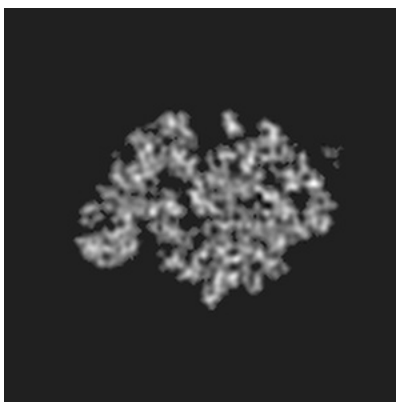
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

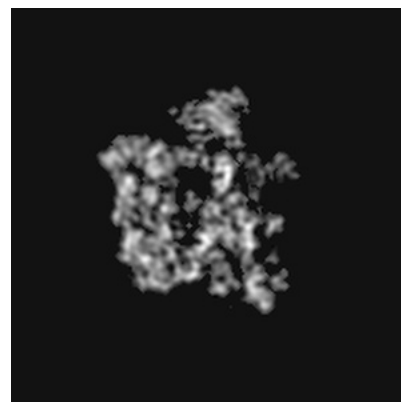
6.2.1 Primary map



X Index: 96



Y Index: 96

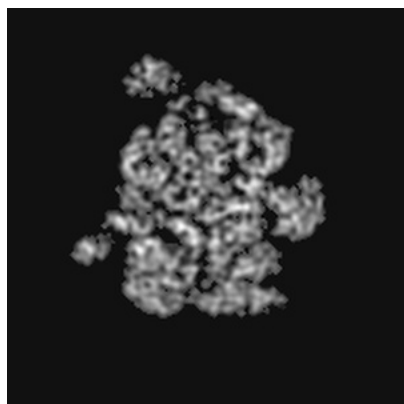


Z Index: 96

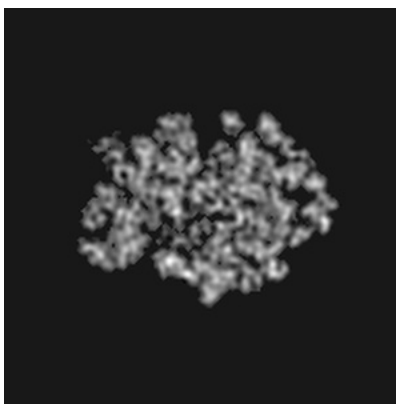
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

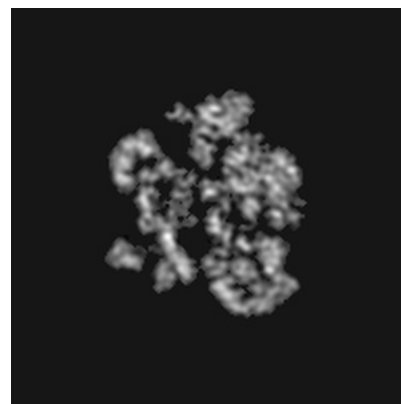
6.3.1 Primary map



X Index: 103



Y Index: 99

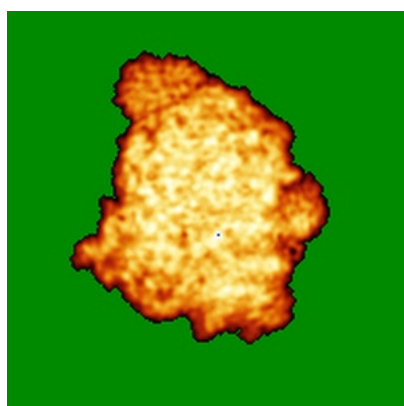


Z Index: 89

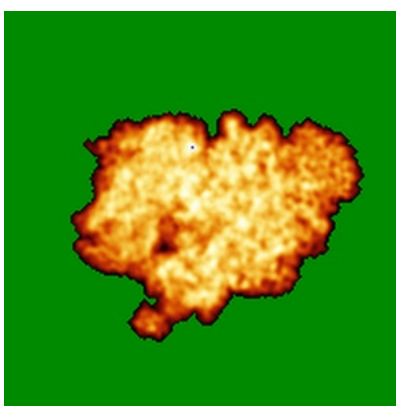
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X



Y



Z

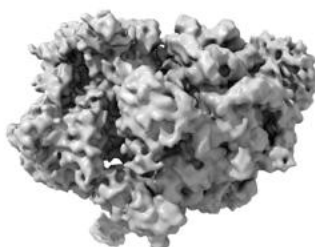
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

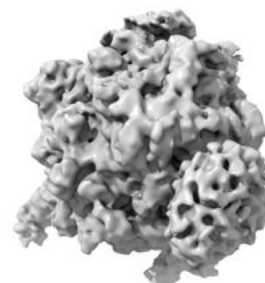
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

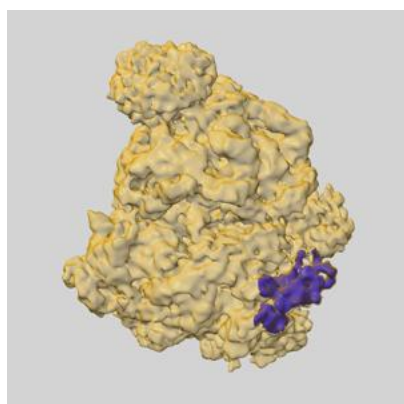
6.6 Mask visualisation [i](#)

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

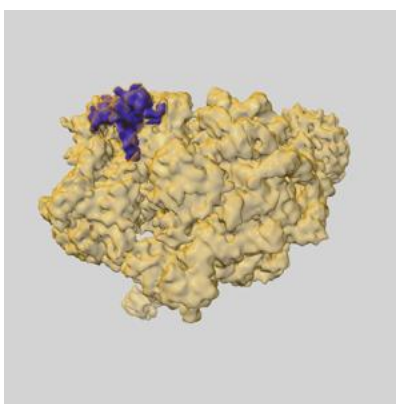
A mask typically either:

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

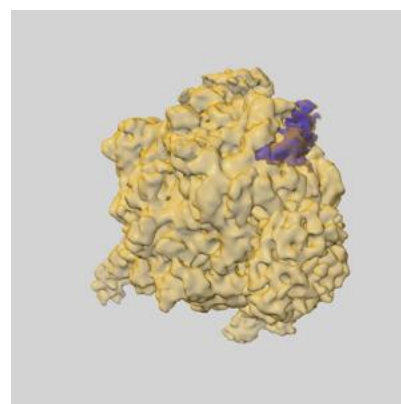
6.6.1 emd_5693_msk_8.map [i](#)



X

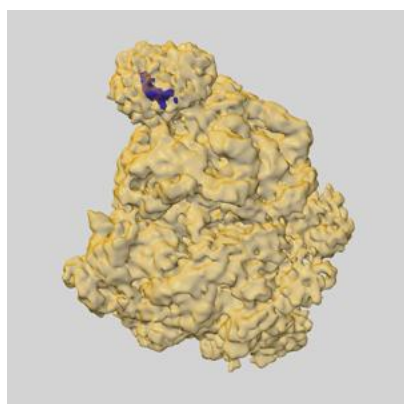


Y

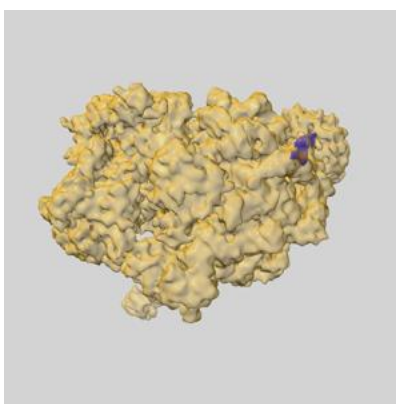


Z

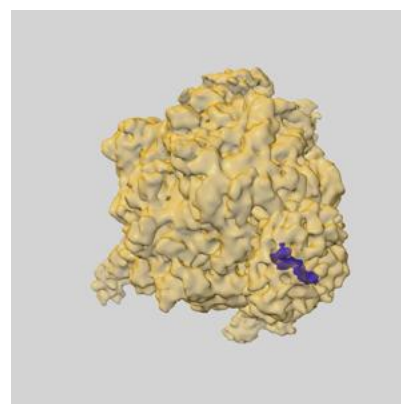
6.6.2 emd_5693_msk_7.map [i](#)



X

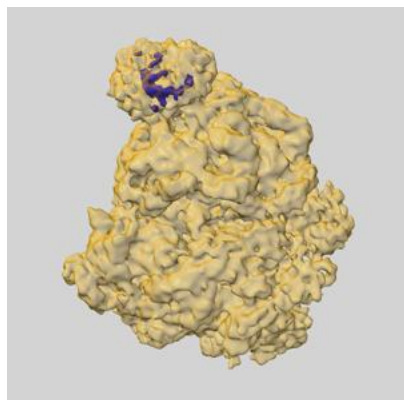


Y

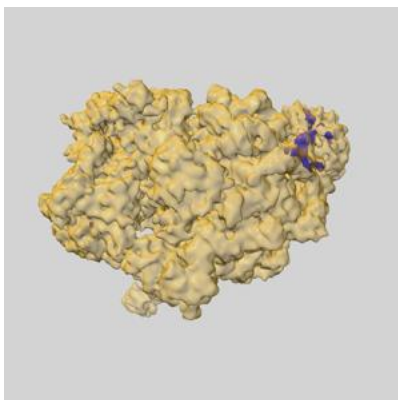


Z

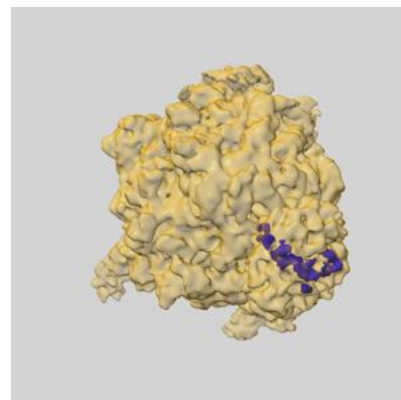
6.6.3 emd_5693_msk_6.map [i](#)



X

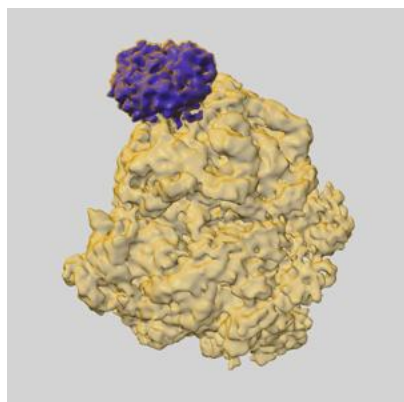


Y

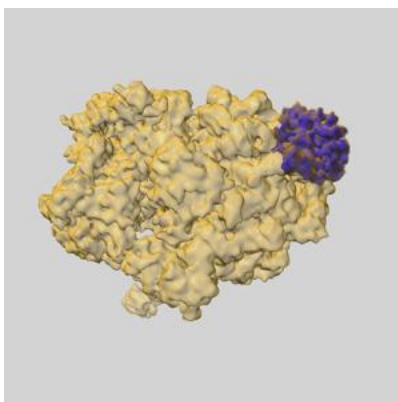


Z

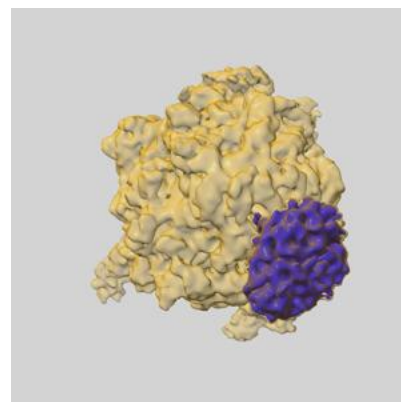
6.6.4 emd_5693_msk_5.map [i](#)



X

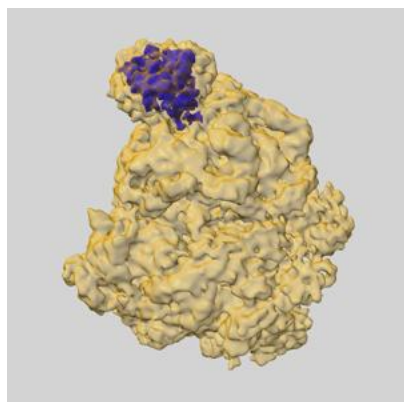


Y

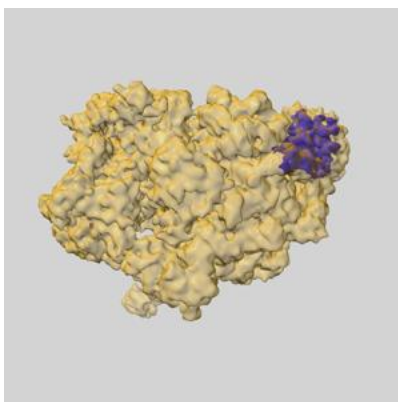


Z

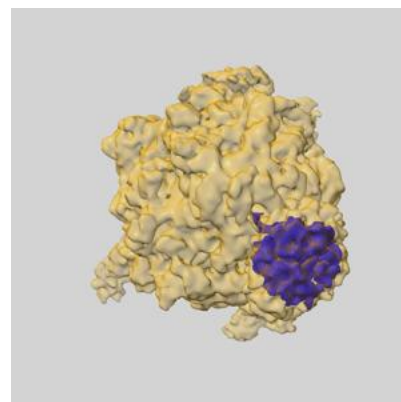
6.6.5 emd_5693_msk_4.map [i](#)



X

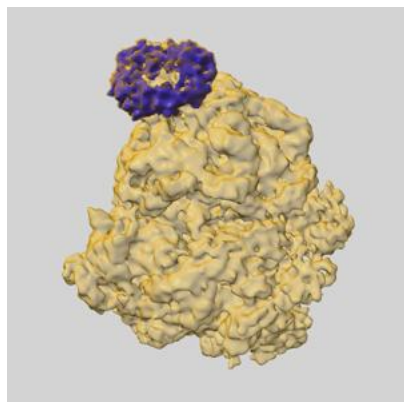


Y

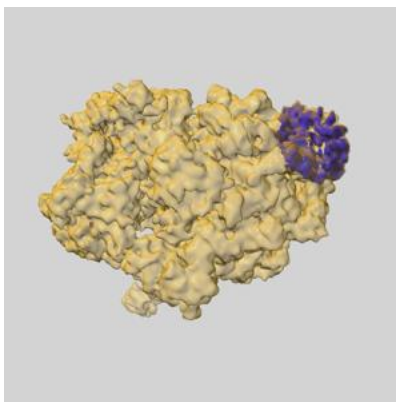


Z

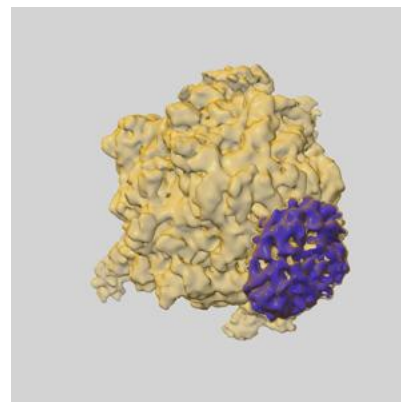
6.6.6 emd_5693_msk_3.map [i](#)



X

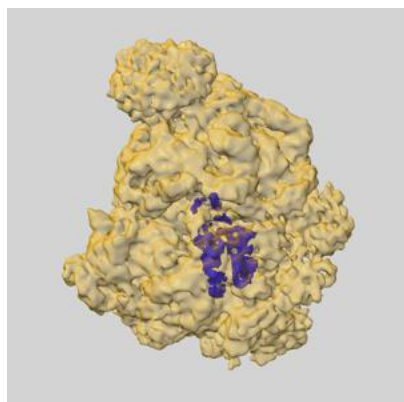


Y

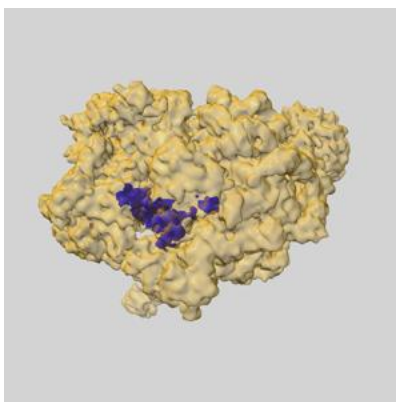


Z

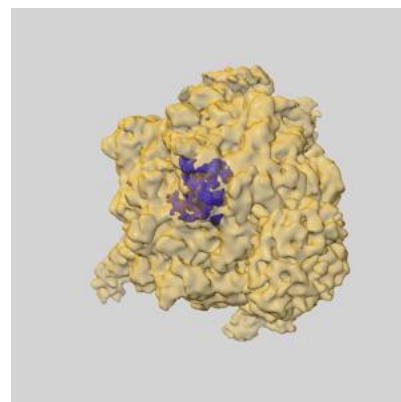
6.6.7 emd_5693_msk_2.map [i](#)



X

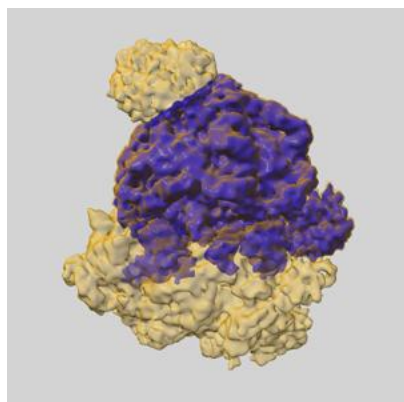


Y

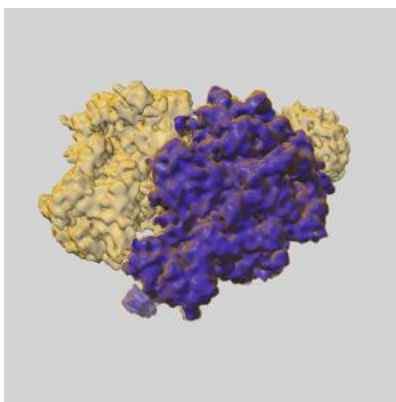


Z

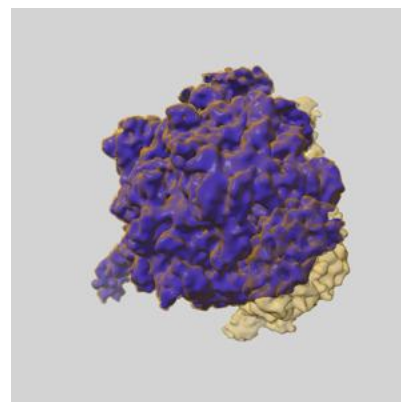
6.6.8 emd_5693_msk_1.map [i](#)



X

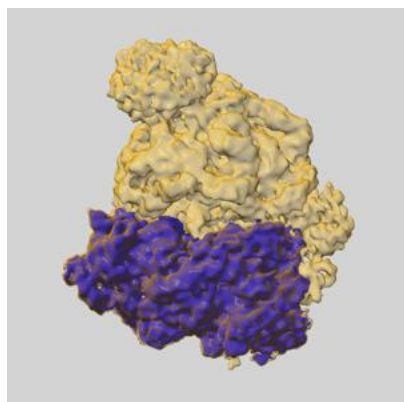


Y

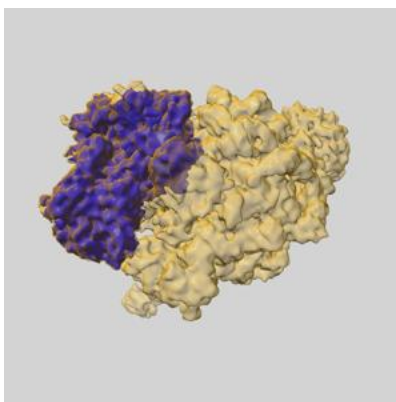


Z

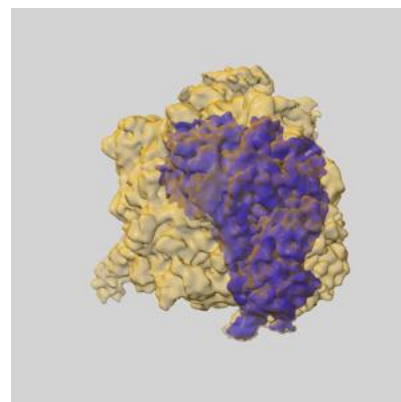
6.6.9 emd_5693_msk_9.map [i](#)



X



Y

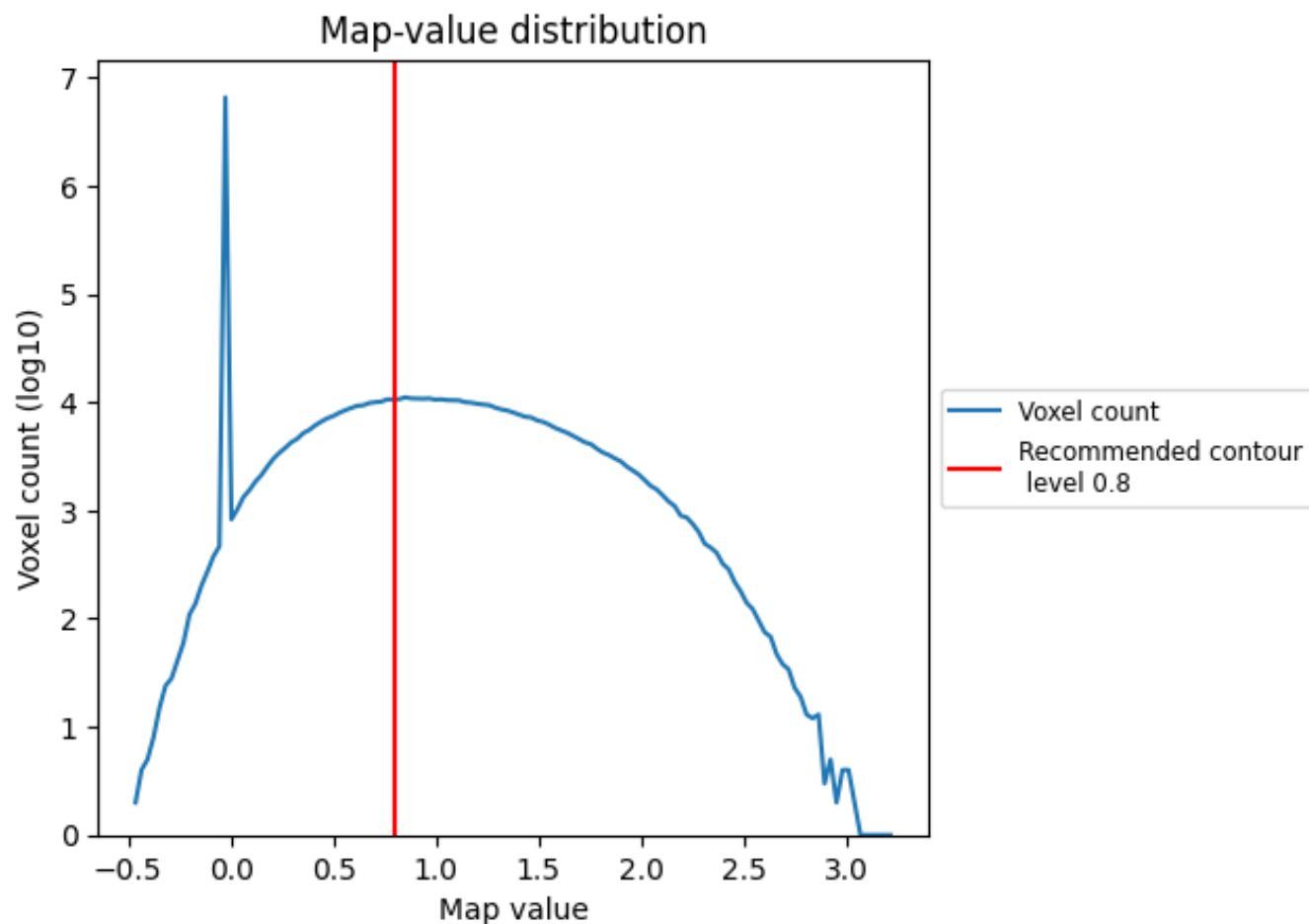


Z

7 Map analysis [i](#)

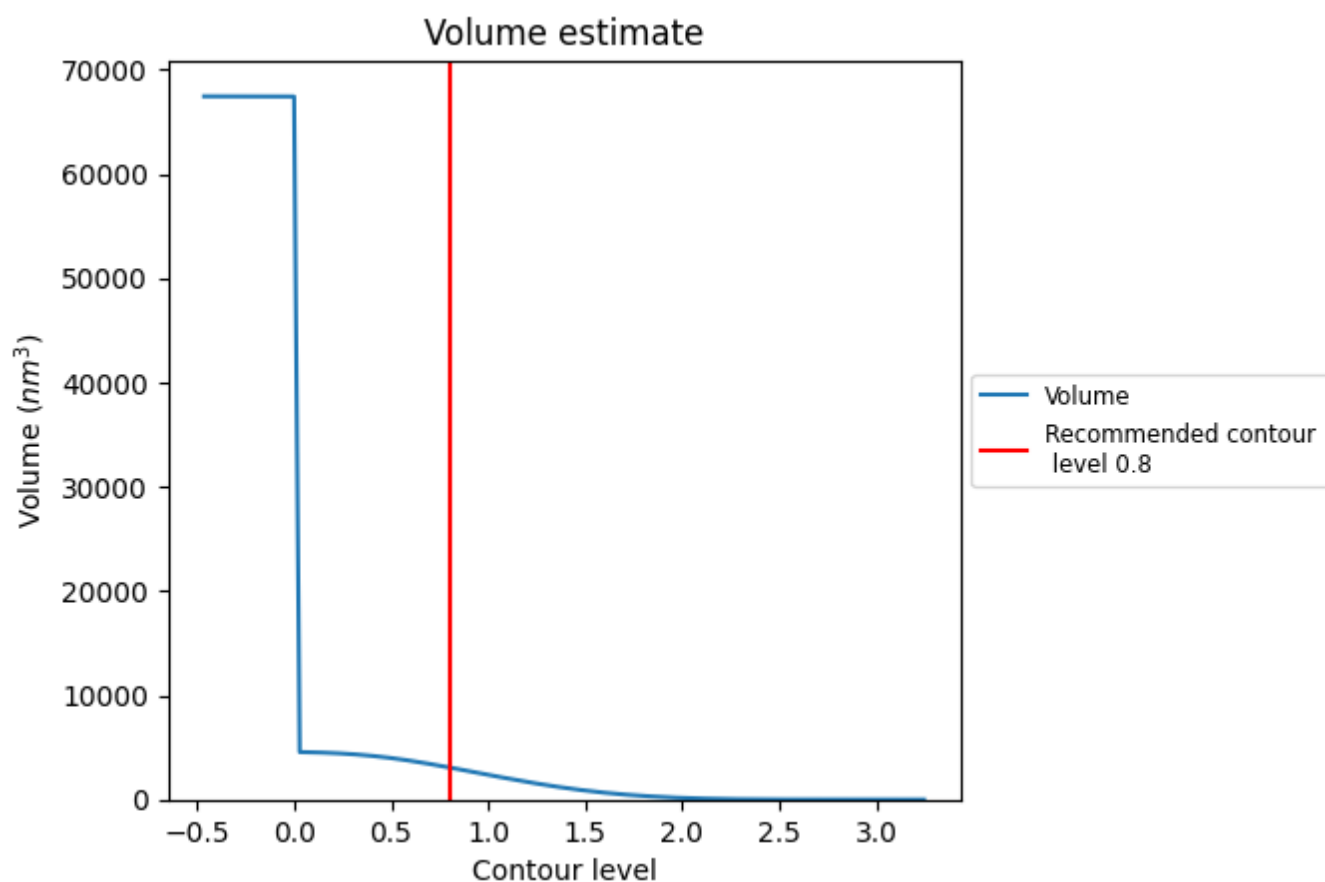
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

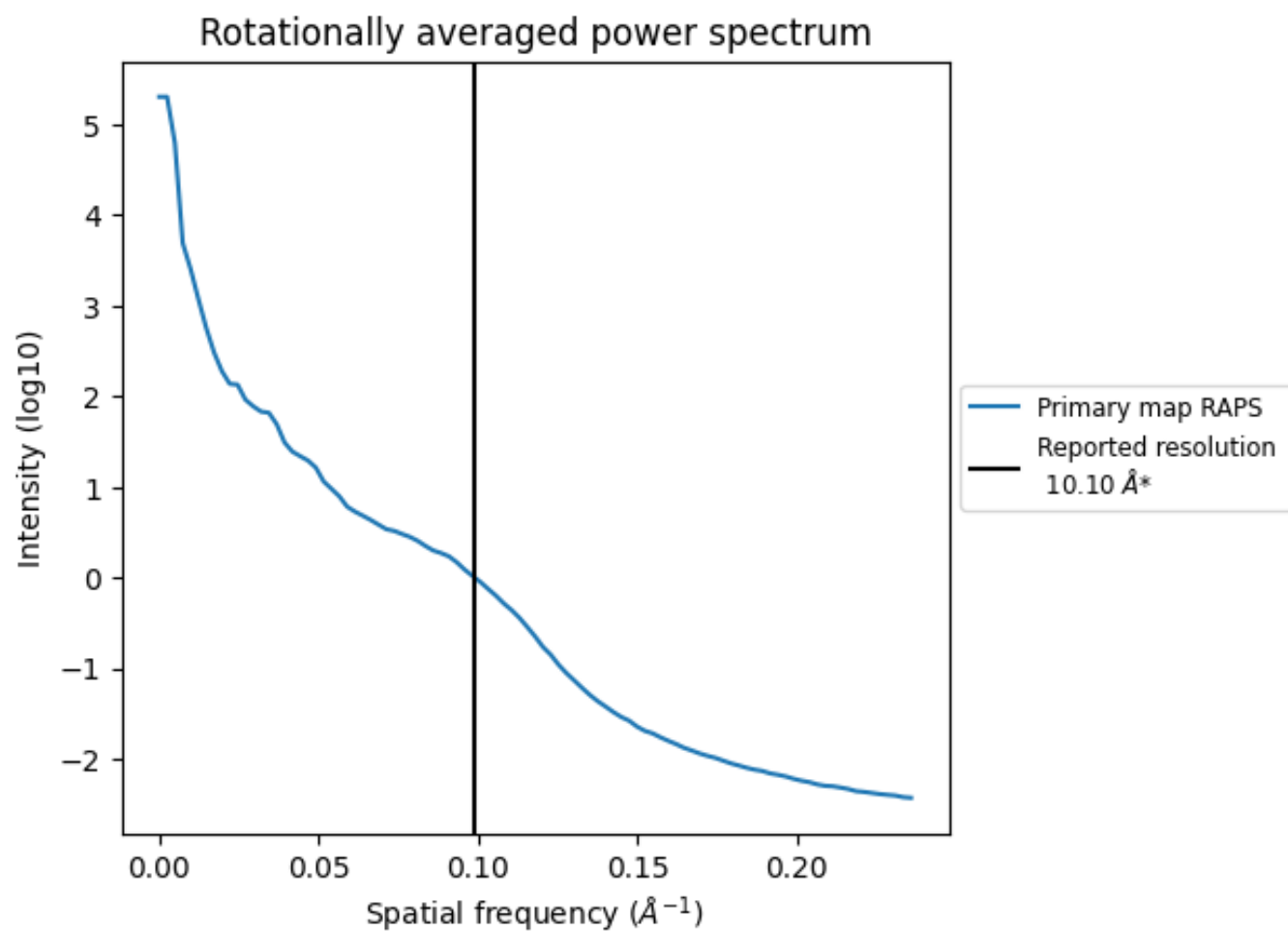
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3075 nm³; this corresponds to an approximate mass of 2778 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 0.099 Å⁻¹

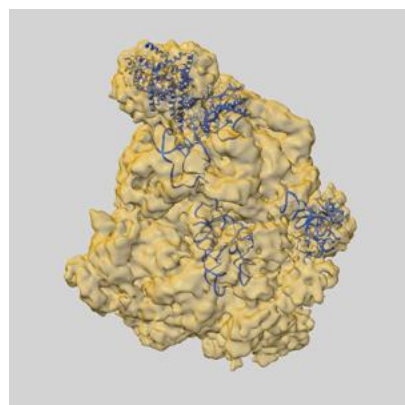
8 Fourier-Shell correlation

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

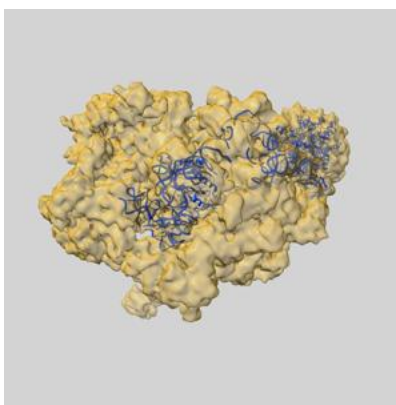
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-5693 and PDB model 3J46. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

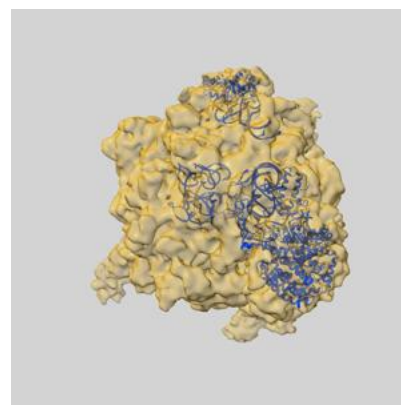
9.1 Map-model overlay [i](#)



X



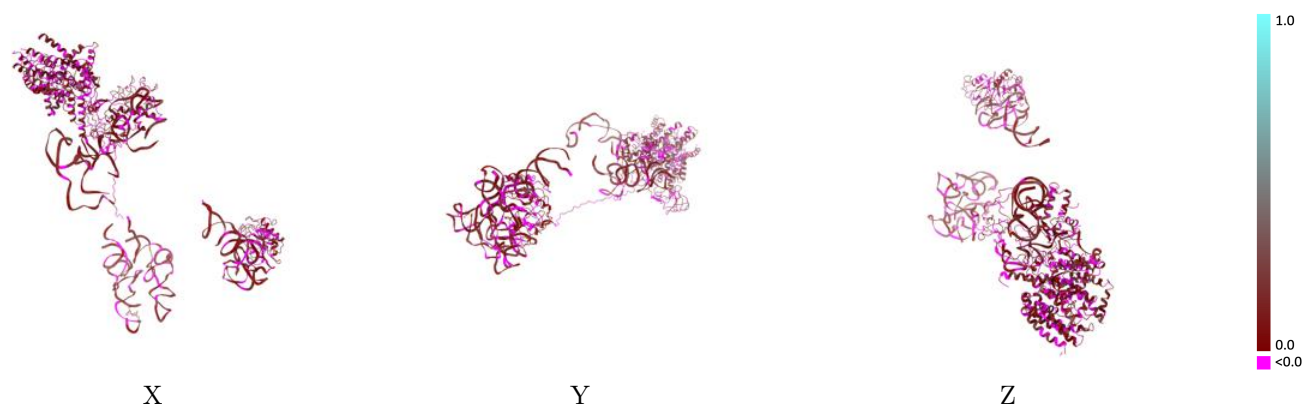
Y



Z

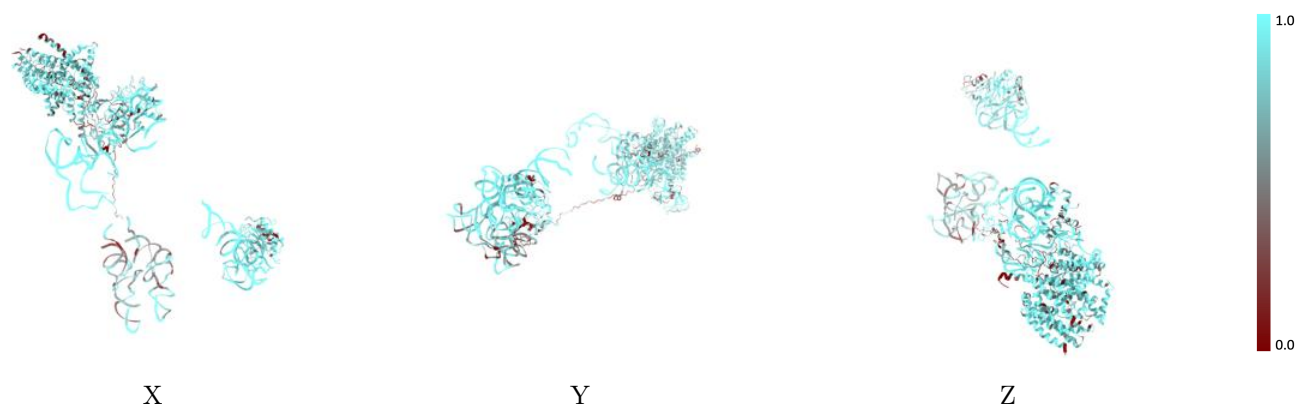
The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



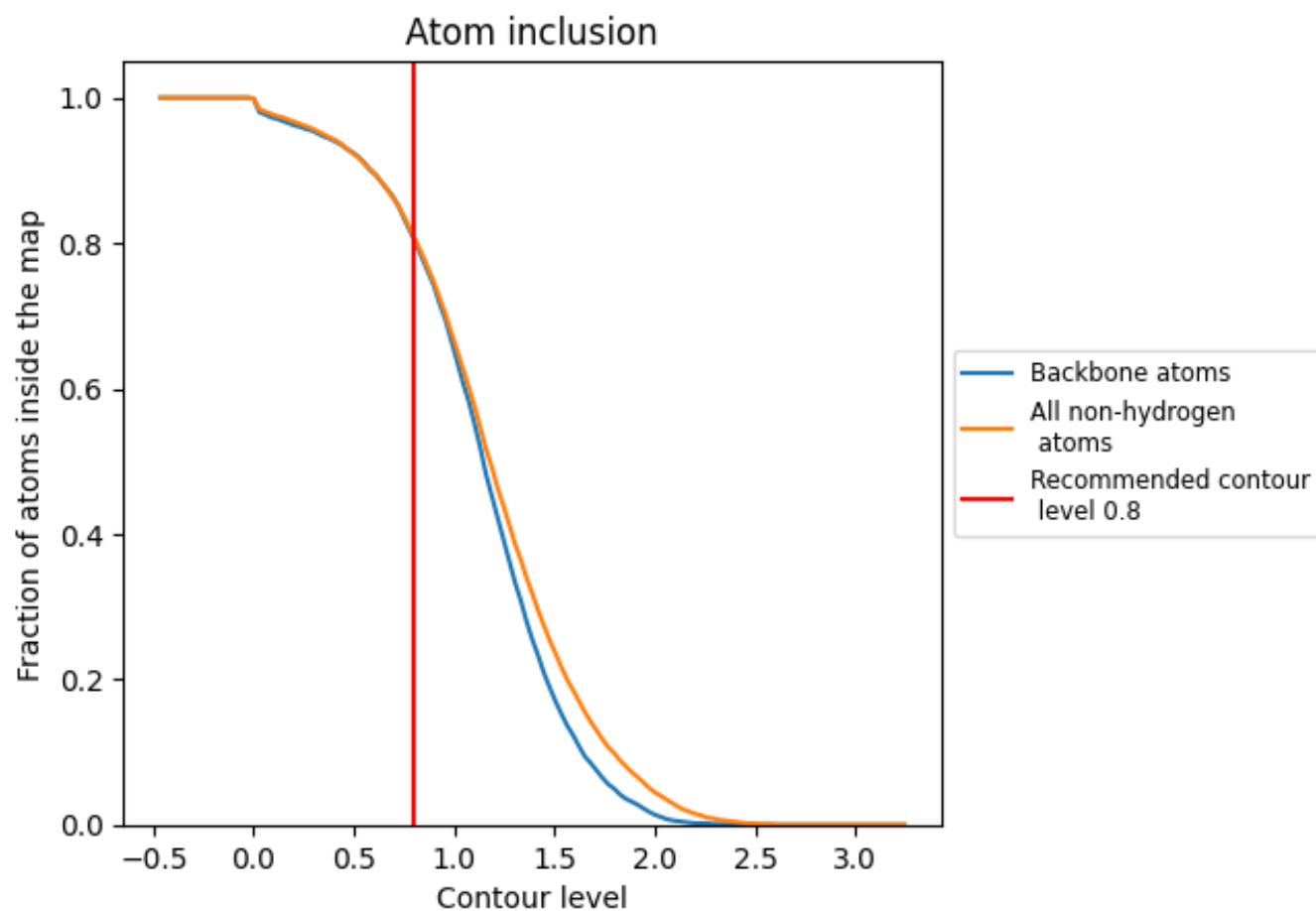
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.8).

9.4 Atom inclusion ⓘ



At the recommended contour level, 80% 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 (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8080	 0.0790
1	 0.9530	 0.1260
2	 0.9550	 0.1000
3	 0.9590	 0.1440
4	 0.9630	 0.0950
5	 0.8070	 0.0590
E	 0.7240	 0.0410
G	 0.8580	 0.0510
T	 0.7280	 0.0700
U	 0.8110	 0.0750
Y	 0.7910	 0.0870
a	 0.6290	 0.0690
n	 0.5290	 -0.0090
p	 0.6580	 0.0960
y	 0.8140	 0.0630

