



Full wwPDB EM Validation Report ⓘ

Dec 21, 2024 – 06:55 am GMT

PDB ID : 9FIA
EMDB ID : EMD-50470
Title : SSU(body) structure derived from the SSU sample of the mitoribosome from *T. gondii*.
Authors : Rocha, R.E.O.; Barua, S.; Boissier, F.; Nguyen, T.T.; Hashem, Y.
Deposited on : 2024-05-28
Resolution : 3.29 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ 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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

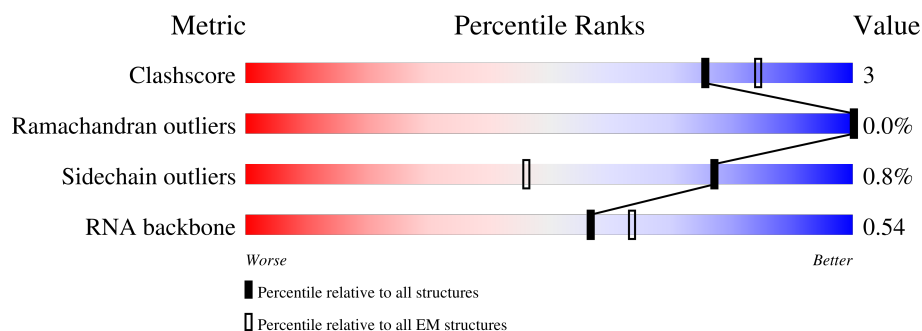
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.29 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	B0	680	<div> <div>11%</div> <div>33%</div> <div>7%</div> <div>59%</div> </div>
2	B1	17	<div> <div>12%</div> <div>100%</div> </div>
3	B2	738	<div> <div>8%</div> <div>40%</div> <div>5%</div> <div>55%</div> </div>
4	B3	377	<div> <div>6%</div> <div>54%</div> <div>42%</div> </div>
5	B4	138	<div> <div>5%</div> <div>53%</div> <div>5%</div> <div>42%</div> </div>
6	B5	393	<div> <div>35%</div> <div>64%</div> </div>
7	B6	163	<div> <div>64%</div> <div>5%</div> <div>31%</div> </div>

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Mol	Chain	Length	Quality of chain
8	B7	12	67% 100%
9	B8	21	24% 100%
9	Bj	21	100%
10	B9	233	25% 73%
11	BA	939	10% 53% 44%
12	BB	1547	13% 30% 6% 65%
13	BC	421	9% 46% 52%
14	BD	686	16% 41% 8% 50%
15	BE	1053	20% 50% 8% 41%
16	BF	304	17% 77% 12% 11%
17	BG	160	14% 89% 8%
18	BH	129	88% 9%
19	BI	13	100%
19	BN	13	15% 100%
19	BX	13	8% 100%
20	BJ	26	27% 100%
21	BK	530	35% 63%
22	BL	116	79% 9% 11%
23	BO	395	63% 35%
24	BP	47	9% 100%
25	BQ	698	8% 59% 6% 35%
26	BS	243	24% 60% 5% 36%
27	BT	280	32% 64%
28	BU	14	29% 100%
29	BV	597	5% 43% 56%

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Mol	Chain	Length	Quality of chain
30	BW	547	
31	BY	11	
32	Ba	10	
33	Bb	8	
34	Bc	716	
35	Bd	33	
36	Be	18	
37	Bg	302	
38	Bh	167	
39	Bi	268	
40	Bk	447	
41	Bl	593	
42	HJ	1140	
43	HS	235	
44	b1	8	
45	b2	48	
46	b3	5	
47	b4	34	
48	bA	34	
49	bD	27	
50	bE	107	
51	bG	4	
52	bH	2	
53	bI	3	
54	bJ	71	

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Mol	Chain	Length	Quality of chain
55	bK	83	
56	bL	48	
57	bN	122	
58	bO	115	
59	bP	15	
60	bQ	14	
61	bR	31	
62	bS	31	
63	bT	60	
64	bU	25	
65	bV	6	
66	bY	11	

2 Entry composition

There are 66 unique types of molecules in this entry. The entry contains 80775 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 Mitochondrial ribosomal protein, mS145.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B0	278	Total	C	N	O	S	0	0
			2311	1461	428	414	8		

- Molecule 2 is a protein called unidentified peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B1	17	Total	C	N	O	0	0
			68	34	17	17		

- Molecule 3 is a protein called Ribosomal protein S18, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B2	335	Total	C	N	O	S	0	0
			2790	1755	522	502	11		

- Molecule 4 is a protein called Mitochondrial ribosomal protein, mS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B3	218	Total	C	N	O	S	0	0
			1735	1092	329	303	11		

- Molecule 5 is a protein called CHCH domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B4	80	Total	C	N	O	S	0	0
			663	434	120	106	3		

- Molecule 6 is a protein called Ribosomal protein S11, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B5	140	Total	C	N	O	S	0	0
			1109	692	229	184	4		

- Molecule 7 is a protein called Putative mitochondrial ribosomal protein s6-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B6	113	Total	C	N	O	S	0	0
			943	606	183	150	4		

- Molecule 8 is a protein called unidentified peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	B7	12	Total	C	N	O	0	0
			48	24	12	12		

- Molecule 9 is a protein called unidentified peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	B8	21	Total	C	N	O	0	0
			84	42	21	21		
9	Bj	21	Total	C	N	O	0	0
			84	42	21	21		

- Molecule 10 is a protein called DnaJ domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B9	62	Total	C	N	O	S	0	0
			531	340	99	91	1		

- Molecule 11 is a protein called Mitochondrial ribosomal protein, mS137.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	BA	526	Total	C	N	O	S	0	0
			4093	2596	723	759	15		

- Molecule 12 is a protein called RAP domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	BB	546	Total	C	N	O	S	0	0
			4313	2744	793	755	21		

- Molecule 13 is a protein called Mitochondrial ribosomal protein, mS47.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	BC	204	Total	C	N	O	S	0	0
			1581	1014	292	269	6		

- Molecule 14 is a protein called Pentatricopeptide repeat domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	BD	341	Total	C	N	O	S	0	0
			2682	1693	498	484	7		

- Molecule 15 is a protein called Mitochondrial ribosomal protein, mS140.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	BE	624	Total	C	N	O	S	0	0
			5085	3236	940	887	22		

- Molecule 16 is a protein called Mitochondrial ribosomal protein, mS147.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	BF	271	Total	C	N	O	S	0	0
			2195	1391	428	370	6		

- Molecule 17 is a protein called Ribosomal protein, uS2m.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	BG	148	Total	C	N	O	S	0	0
			1187	765	210	204	8		

- Molecule 18 is a protein called Putative ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	BH	125	Total	C	N	O	S	0	0
			998	636	188	166	8		

- Molecule 19 is a protein called unidentified peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	BI	13	Total	C	N	O	0	0
			52	26	13	13		
19	BN	13	Total	C	N	O	0	0
			52	26	13	13		
19	BX	13	Total	C	N	O	0	0
			52	26	13	13		

- Molecule 20 is a protein called unidentified peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	BJ	26	Total	C	N	O	0	0
			104	52	26	26		

- Molecule 21 is a protein called Mitochondrial ribosomal protein, mS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	BK	198	Total	C	N	O	S	0	0
			1673	1068	307	292	6		

- Molecule 22 is a protein called Putative ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BL	103	Total	C	N	O	S	0	0
			887	570	168	144	5		

- Molecule 23 is a protein called Putative 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	BO	257	Total	C	N	O	S	0	0
			2150	1371	419	350	10		

- Molecule 24 is a protein called unidentified peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	BP	47	Total	C	N	O	0	0
			188	94	47	47		

- Molecule 25 is a protein called Macro domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BQ	455	Total	C	N	O	S	0	0
			3588	2295	657	628	8		

- Molecule 26 is a protein called Ribosomal protein, bS21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BS	156	Total	C	N	O	S	0	0
			1305	825	253	225	2		

- Molecule 27 is a protein called Mitochondrial ribosomal protein, mS156.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BT	100	Total	C	N	O	S	0	0
			801	519	148	132	2		

- Molecule 28 is a protein called unidentified peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	BU	14	Total	C	N	O	0	0
			56	28	14	14		

- Molecule 29 is a protein called Putative homeodomain containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BV	262	Total	C	N	O	S	0	0
			2181	1410	370	395	6		

- Molecule 30 is a protein called Mitochondrial ribosomal protein, mS144.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	BW	339	Total	C	N	O	S	0	0
			2716	1714	489	503	10		

- Molecule 31 is a protein called unidentified peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	BY	11	Total	C	N	O	0	0
			44	22	11	11		

- Molecule 32 is a protein called unidentified peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	Ba	10	Total	C	N	O	0	0
			40	20	10	10		

- Molecule 33 is a protein called unidentified peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	Bb	8	Total	C	N	O	0	0
			32	16	8	8		

- Molecule 34 is a protein called Enoyl-CoA hydratase/isomerase family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Bc	537	Total	C	N	O	S	0	0
			4276	2717	763	779	17		

- Molecule 35 is a protein called unidentified peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	Bd	33	Total	C	N	O	0	0
			132	66	33	33		

- Molecule 36 is a protein called unidentified peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	Be	18	Total	C	N	O	0	0
			72	36	18	18		

- Molecule 37 is a protein called Ribosomal protein, uS2m.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Bg	187	Total	C	N	O	S	0	0
			1543	997	294	249	3		

- Molecule 38 is a protein called Putative 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Bh	153	Total	C	N	O	S	0	0
			1242	791	229	215	7		

- Molecule 39 is a protein called Mitochondrial ribosomal protein, mS153.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Bi	119	Total	C	N	O	S	0	0
			928	595	163	167	3		

- Molecule 40 is a protein called Mitochondrial ribosomal protein, mS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Bk	415	Total	C	N	O	S	0	0
			3394	2130	645	612	7		

- Molecule 41 is a protein called 30S ribosomal protein S12, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Bl	200	Total	C	N	O	S	0	0
			1660	1044	334	276	6		

- Molecule 42 is a protein called 30S ribosomal protein S5, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	HJ	355	Total	C	N	O	S	0	0
			2916	1851	550	505	10		

- Molecule 43 is a protein called Acylphosphatase-like domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	HS	90	Total	C	N	O	S	0	0
			720	450	141	127	2		

- Molecule 44 is a RNA chain called ulr11.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	b1	8	Total	C	N	O	P	0	0
			160	72	16	64	8		

- Molecule 45 is a RNA chain called SSUE.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	b2	30	Total	C	N	O	P	0	0
			632	284	112	206	30		

- Molecule 46 is a RNA chain called ulr12.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	b3	5	Total	C	N	O	P	0	0
			100	45	10	40	5		

- Molecule 47 is a RNA chain called RNA13.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	b4	27	Total	C	N	O	P	0	0
			585	260	108	190	27		

- Molecule 48 is a RNA chain called RNA19.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	bA	27	Total	C	N	O	P	0	0
			571	255	93	196	27		

- Molecule 49 is a RNA chain called RNA15.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	bD	25	Total	C	N	O	P	0	0
			546	243	106	172	25		

- Molecule 50 is a RNA chain called RNA8.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	bE	92	Total	C	N	O	P	0	0
			1965	879	355	639	92		

- Molecule 51 is a RNA chain called ulr13.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	bG	4	Total	C	N	O	P	0	0
			80	36	8	32	4		

- Molecule 52 is a RNA chain called ulr14.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	bH	2	Total	C	N	O	P	0	0
			40	18	4	16	2		

- Molecule 53 is a RNA chain called ulr15.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	bI	3	Total	C	N	O	P	0	0
			60	27	6	24	3		

- Molecule 54 is a RNA chain called RNA33.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	bJ	58	Total	C	N	O	P	0	0
			1220	548	203	411	58		

- Molecule 55 is a RNA chain called RNA5.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	bK	66	Total	C	N	O	P	0	0
			1397	628	246	457	66		

- Molecule 56 is a RNA chain called RNA17.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	bL	48	Total	C	N	O	P	0	0
			1019	456	176	339	48		

- Molecule 57 is a RNA chain called SSUB.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	bN	50	Total	C	N	O	P	0	0
			1069	477	187	355	50		

- Molecule 58 is a RNA chain called SSUA.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	bO	115	Total	C	N	O	P	0	0
			2451	1099	445	792	115		

- Molecule 59 is a RNA chain called ulr16.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	bP	15	Total	C	N	O	P	0	0
			300	135	30	120	15		

- Molecule 60 is a RNA chain called ulr17.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	bQ	14	Total	C	N	O	P	0	0
			280	126	28	112	14		

- Molecule 61 is a RNA chain called RNA30.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	bR	19	Total	C	N	O	P	0	0
			408	183	77	129	19		

- Molecule 62 is a RNA chain called url18.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	bS	31	Total	C	N	O	P	0	0
			620	279	62	248	31		

- Molecule 63 is a RNA chain called SSUF.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	bT	52	Total	C	N	O	P	0	0
			1128	504	219	353	52		

- Molecule 64 is a RNA chain called ulr19.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	bU	25	Total	C	N	O	P	0	0
			500	225	50	200	25		

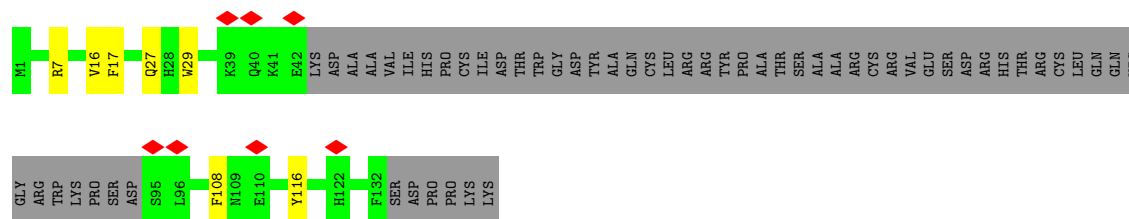
- Molecule 65 is a RNA chain called ulr20.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	bV	6	Total	C	N	O	P	0	0
			120	54	12	48	6		

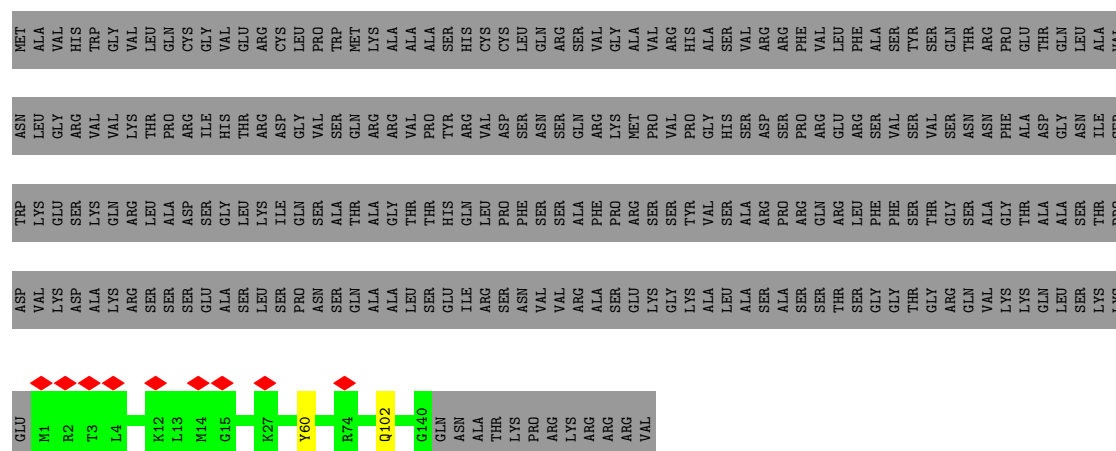
- Molecule 66 is a RNA chain called ulr21.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	bY	11	Total	C	N	O	P	0	0
			220	99	22	88	11		

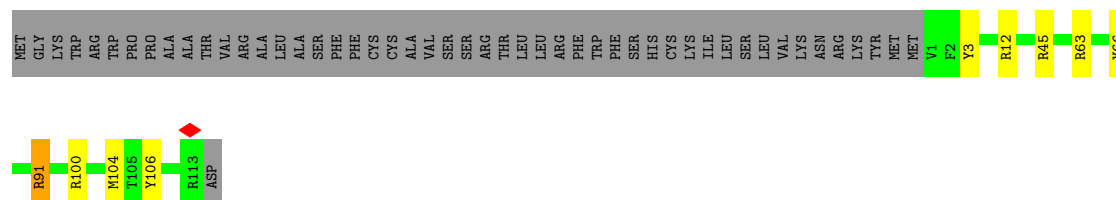
- Molecule 5: CHCH domain-containing protein



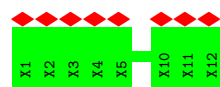
- Molecule 6: Ribosomal protein S11, putative



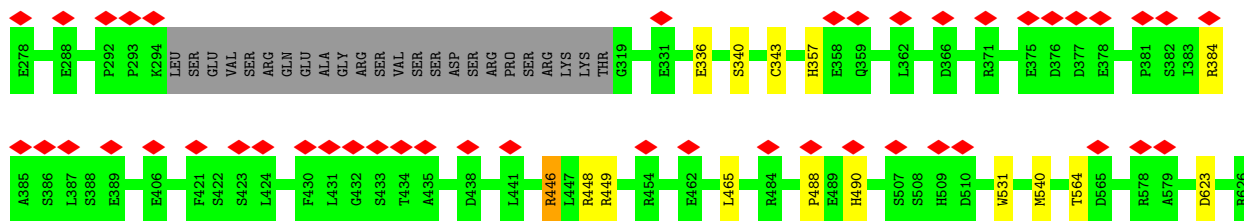
- Molecule 7: Putative mitochondrial ribosomal protein s6-2



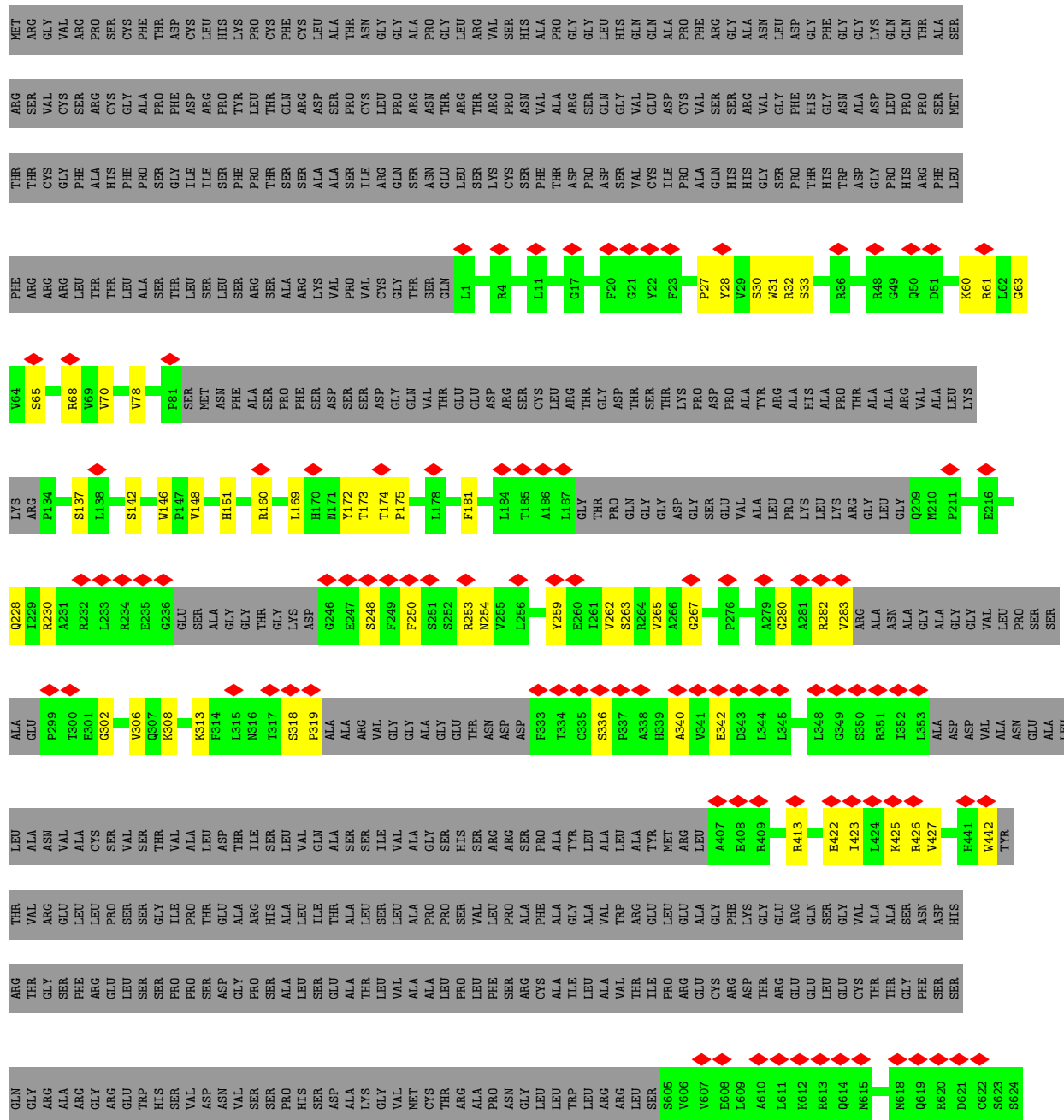
- Molecule 8: unidentified peptide



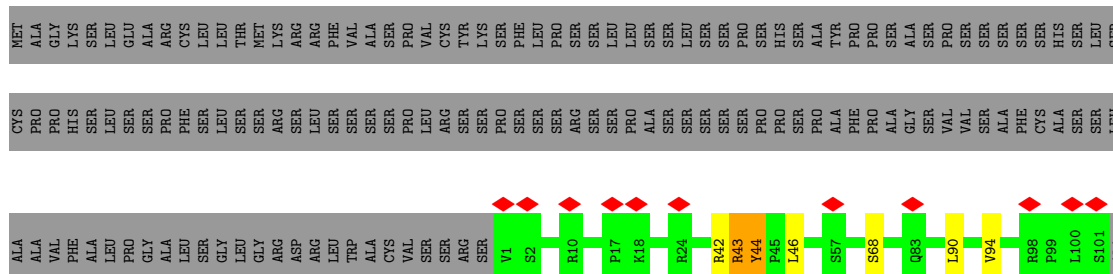
- Molecule 9: unidentified peptide

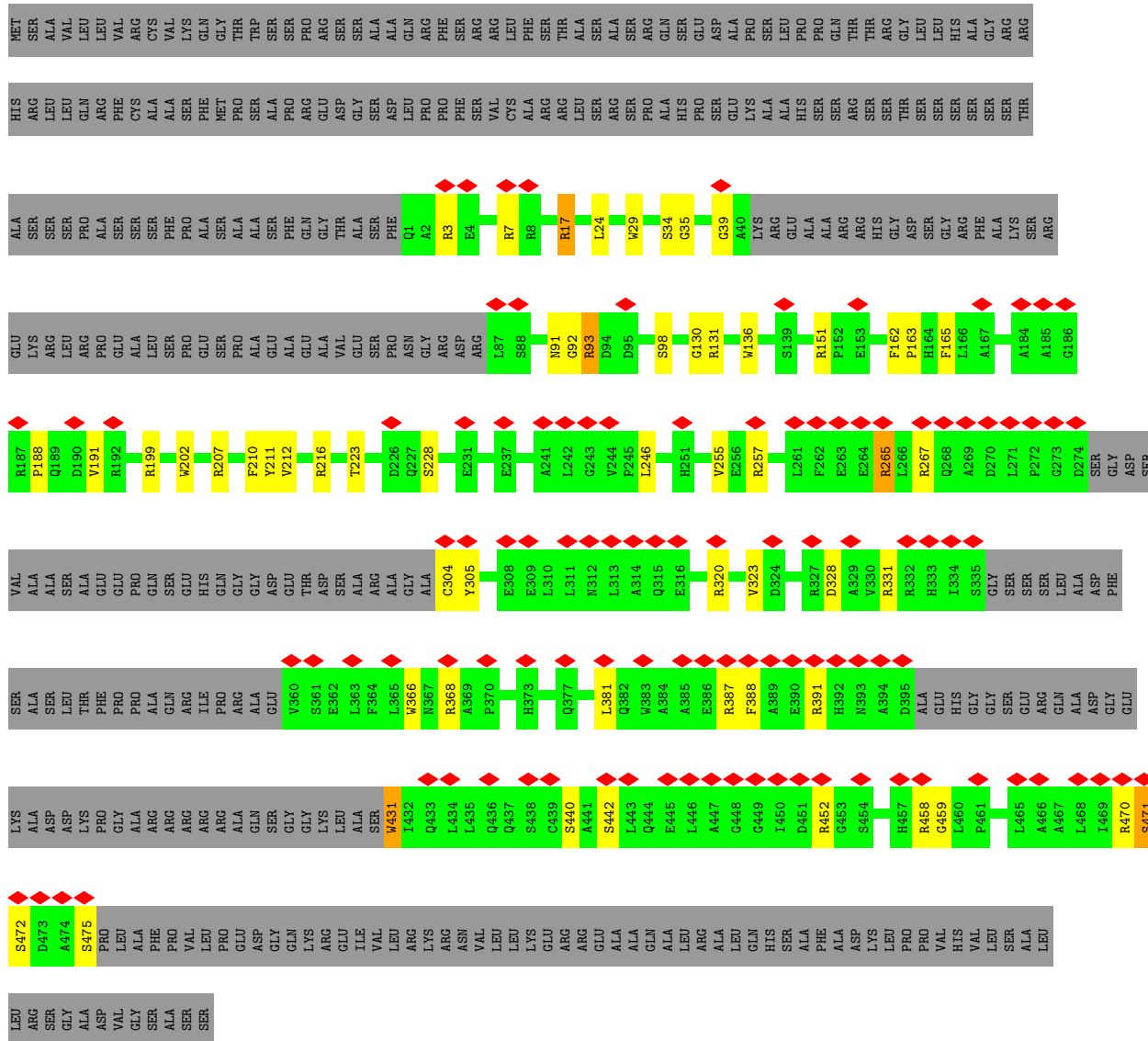


• Molecule 12: RAP domain-containing protein

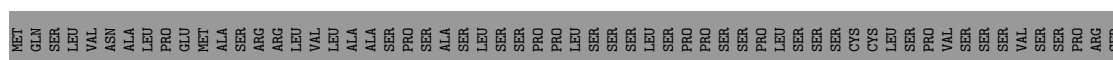


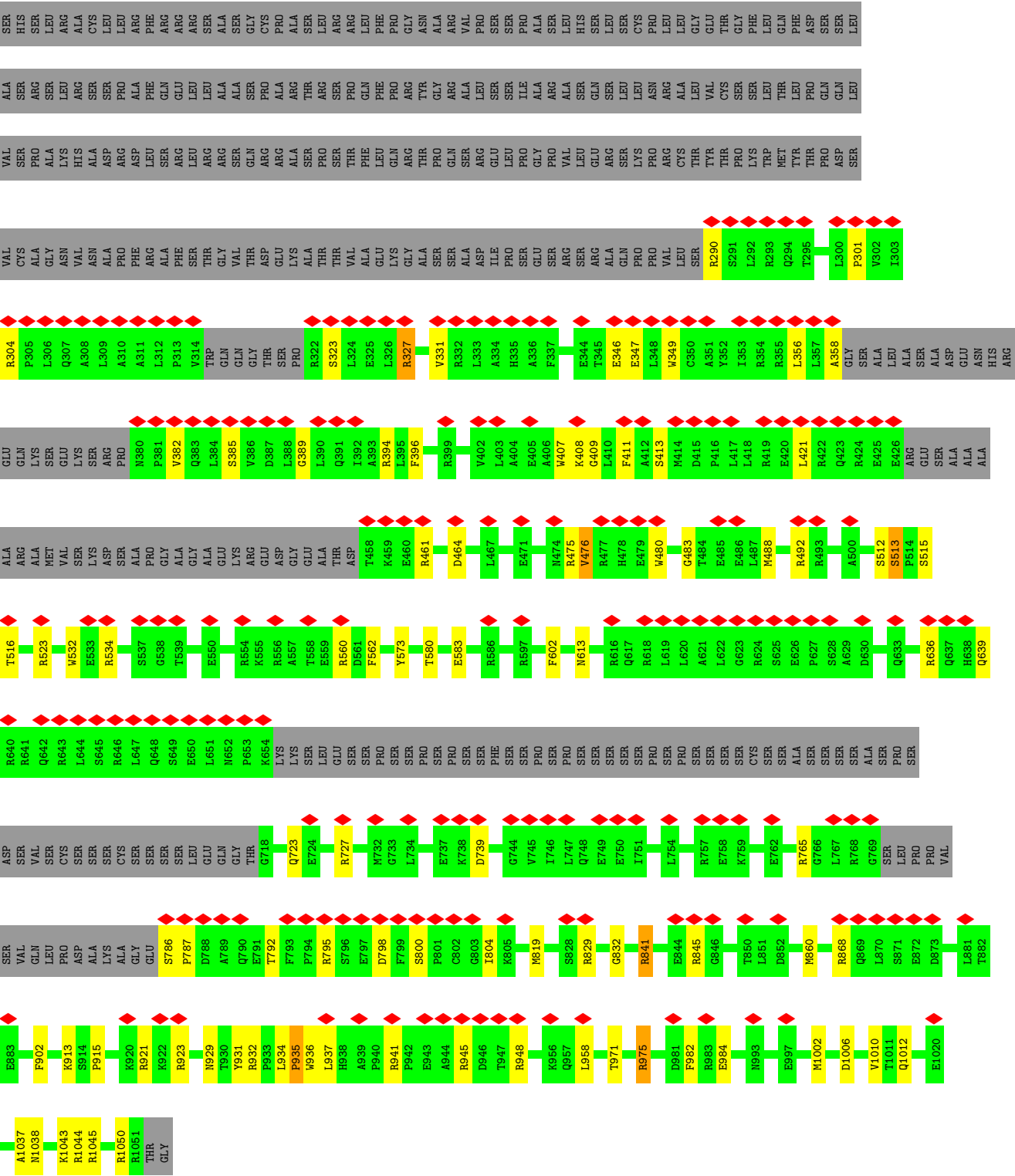
- Molecule 13: Mitochondrial ribosomal protein, mS47



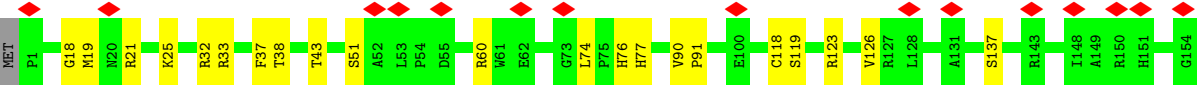
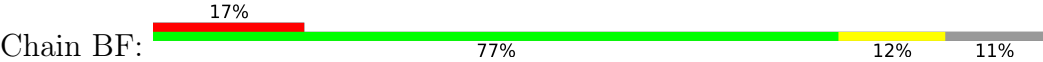


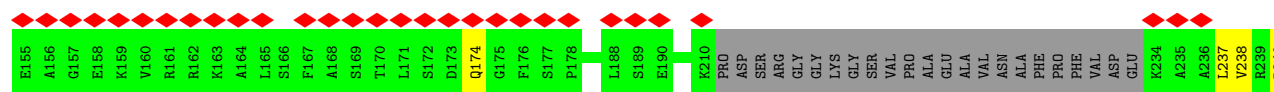
- Molecule 15: Mitochondrial ribosomal protein, mS140



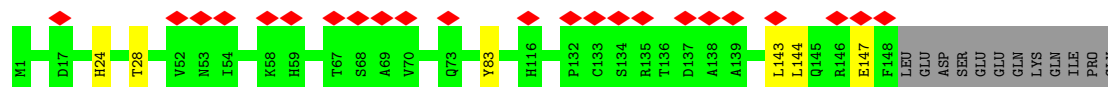
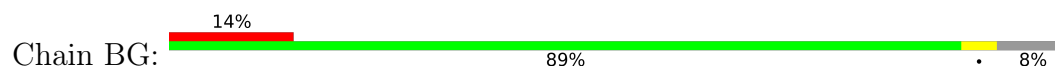


● Molecule 16: Mitochondrial ribosomal protein, mS147





- Molecule 17: Ribosomal protein, uS2m



- Molecule 18: Putative ribosomal protein S8

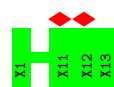


- Molecule 19: unidentified peptide

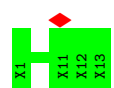


There are no outlier residues recorded for this chain.

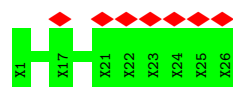
- Molecule 19: unidentified peptide



- Molecule 19: unidentified peptide



- Molecule 20: unidentified peptide



- Molecule 22: Putative ribosomal protein S17

MET	ALA	ASN	SER	THR	LEU	LEU	HIS	TRP	H1	D33	D44	R45	D75	R78	Y84	R85	I86	G87	Y92	R96	E101	F102	R103	ASP
-----	-----	-----	-----	-----	-----	-----	-----	-----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	-----

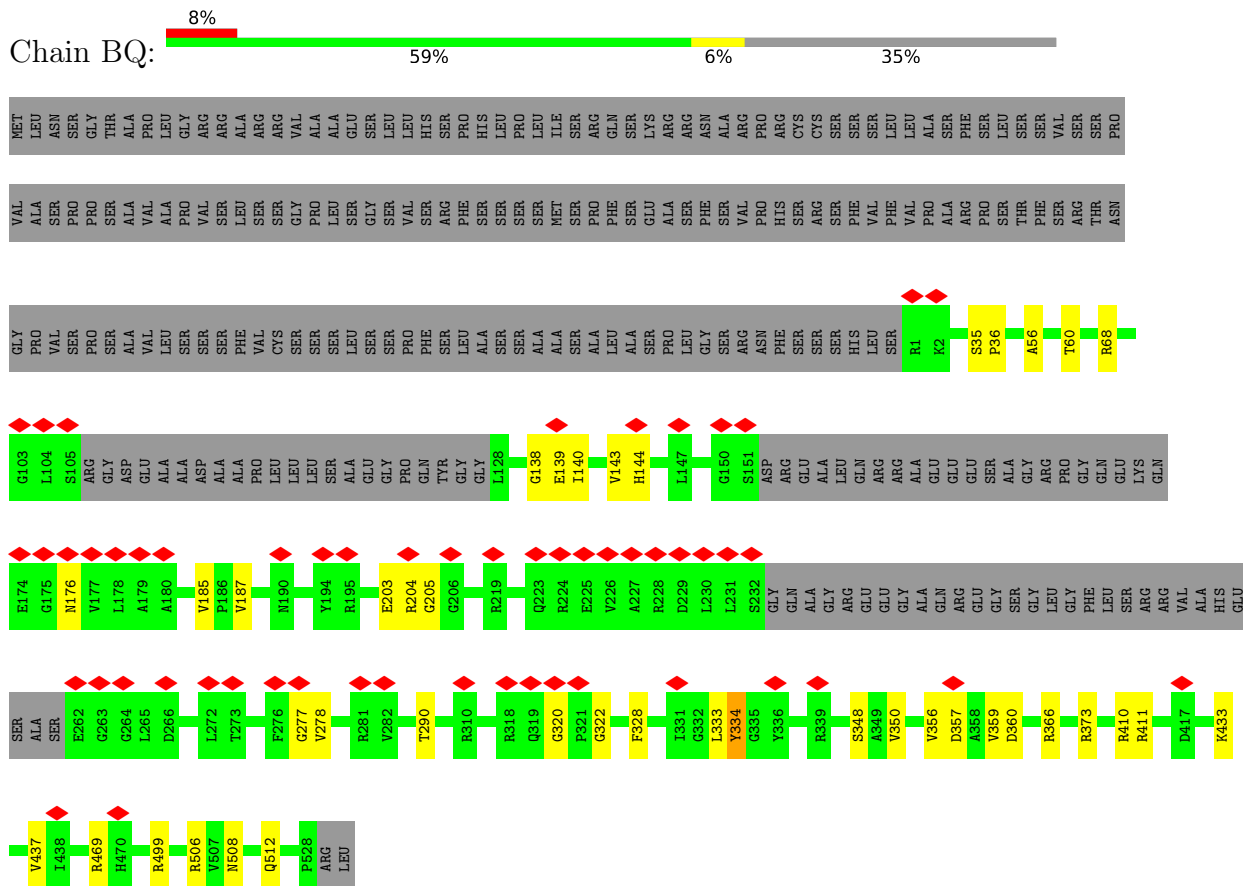
- Molecule 23: Putative 30S ribosomal protein S15

[illegible]

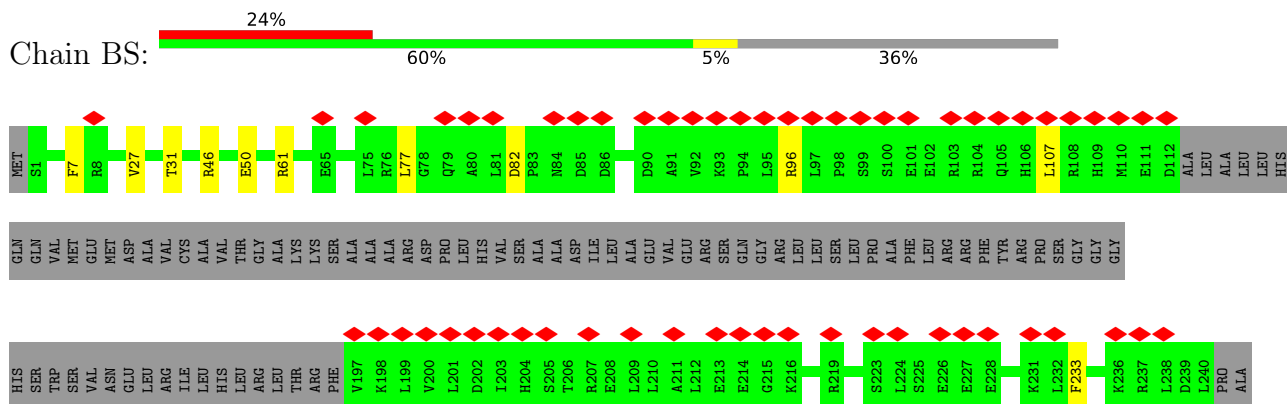
- Molecule 24: unidentified peptide

Diagram illustrating a sequence of nodes: X1, X5, X29, X46, and X47. The nodes are connected in a sequence: X1 to X5, X5 to X29, and X29 to X46. X46 and X47 are connected by a double line. Red diamonds are placed above X5, X29, X46, and X47.

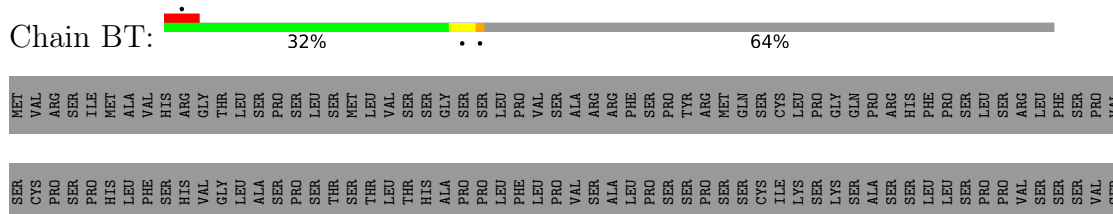
- Molecule 25: Macro domain-containing protein

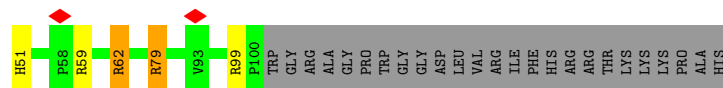


- Molecule 26: Ribosomal protein, bS21m

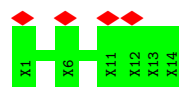


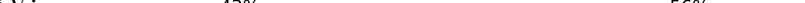
- Molecule 27: Mitochondrial ribosomal protein, mS156

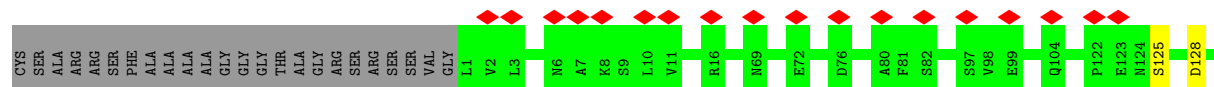
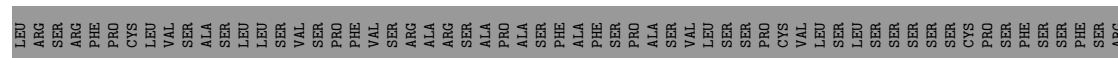
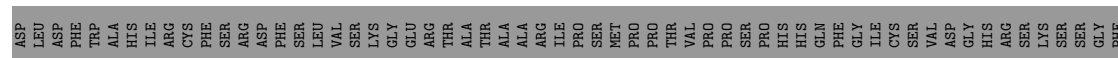
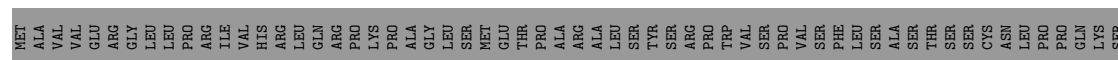




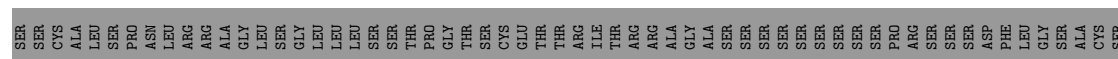
- Chain BU: 

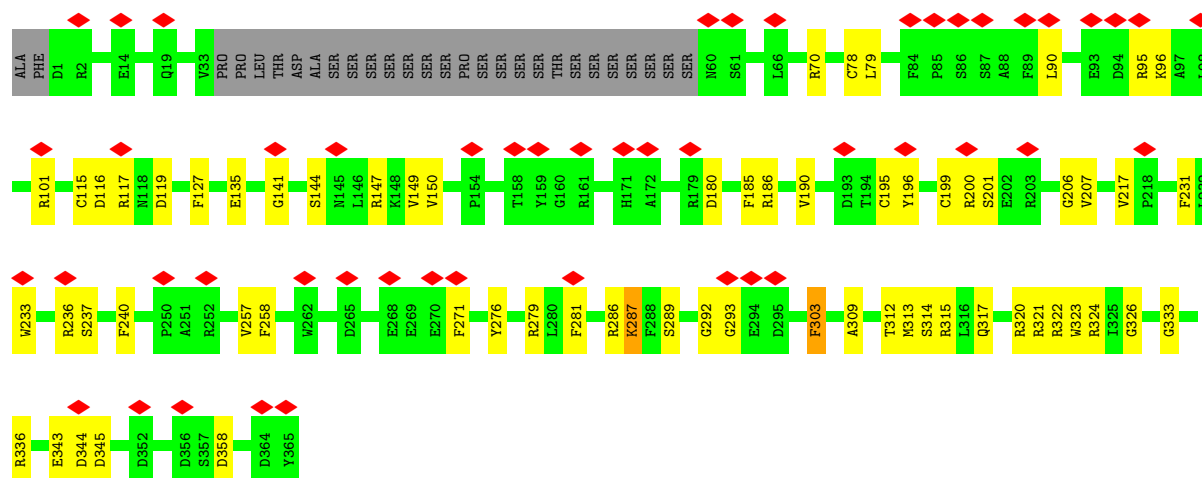


- Chain BV: 

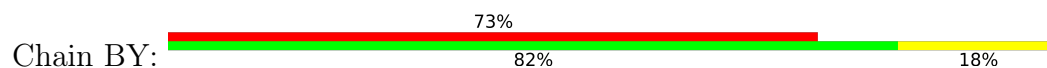


- Chain BW: 

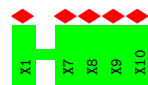




- Molecule 31: unidentified peptide



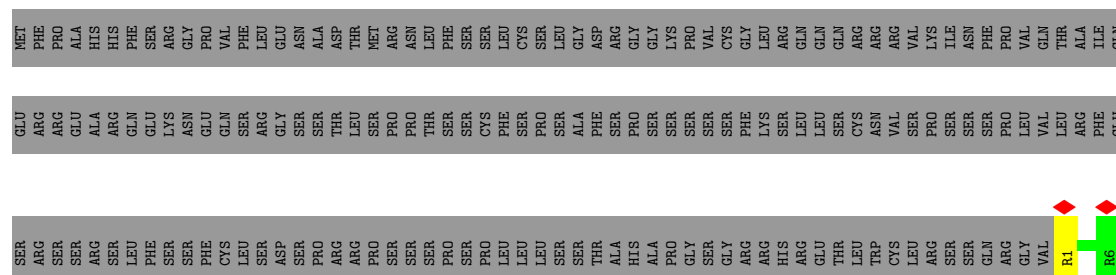
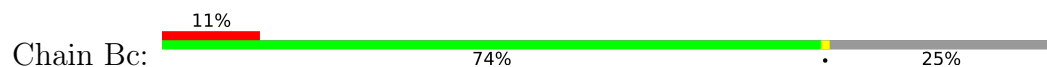
- Molecule 32: unidentified peptide

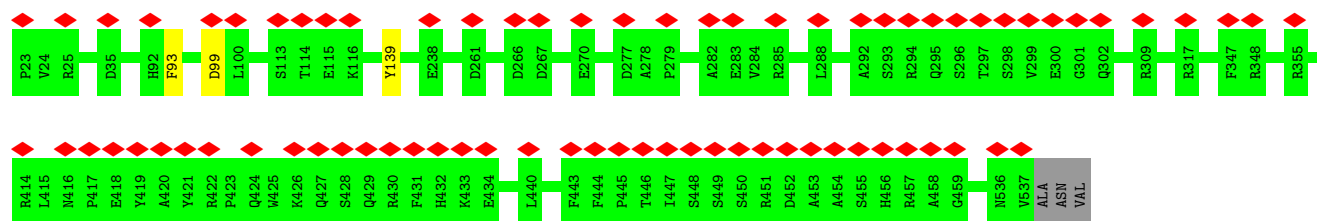


- Molecule 33: unidentified peptide

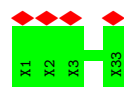


- Molecule 34: Enoyl-CoA hydratase/isomerase family protein





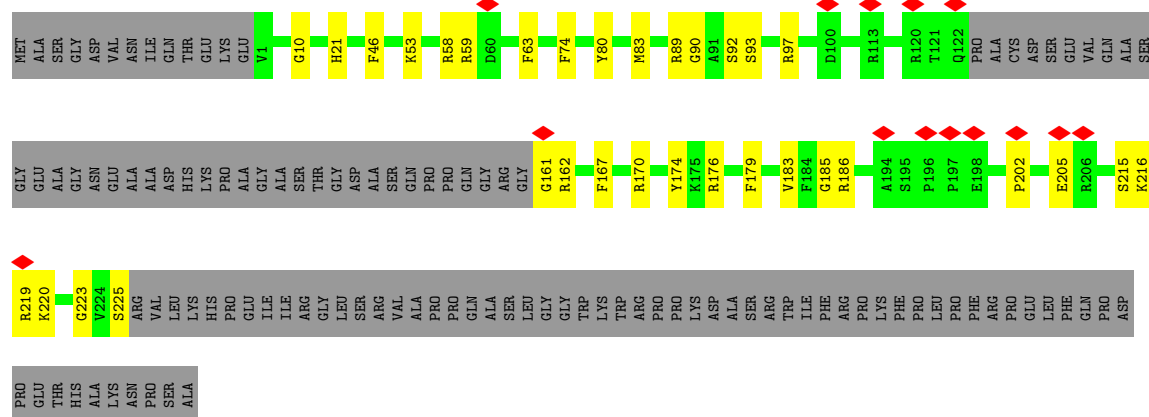
- Molecule 35: unidentified peptide



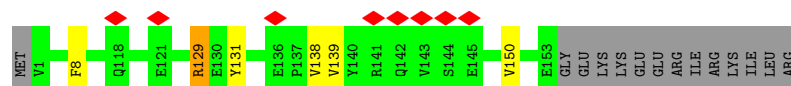
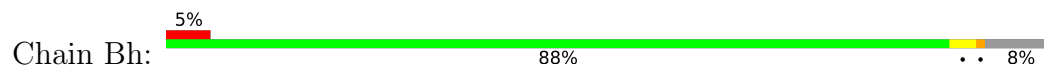
- Molecule 36: unidentified peptide



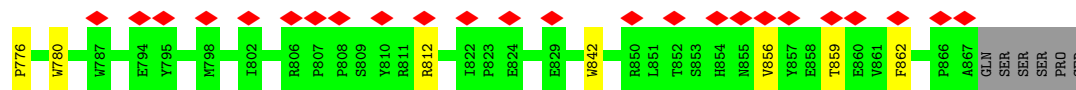
- Molecule 37: Ribosomal protein, uS2m



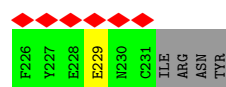
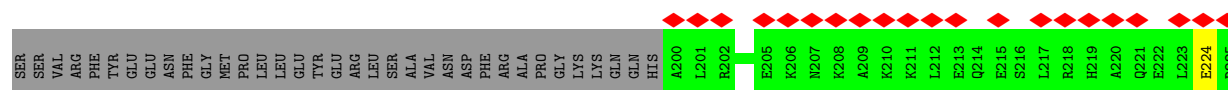
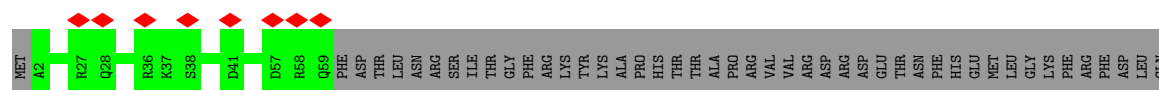
- Molecule 38: Putative 30S ribosomal protein S16



- Molecule 39: Mitochondrial ribosomal protein, mS153



- Molecule 43: Acylphosphatase-like domain-containing protein



- Molecule 44: ulr11

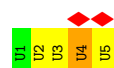


There are no outlier residues recorded for this chain.

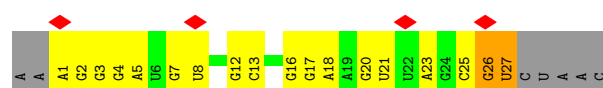
- Molecule 45: SSUE



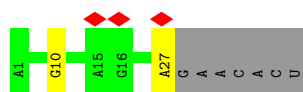
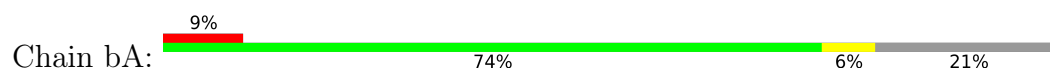
- Molecule 46: ulr12



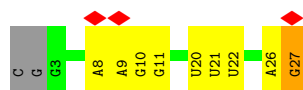
- Molecule 47: RNA13



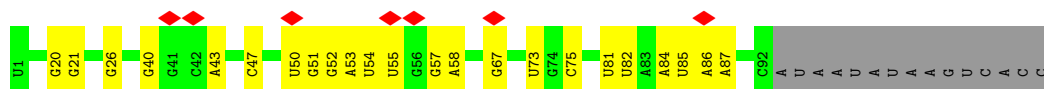
- Molecule 48: RNA19



- Molecule 49: RNA15



- Molecule 50: RNA8



- Molecule 51: ulr13



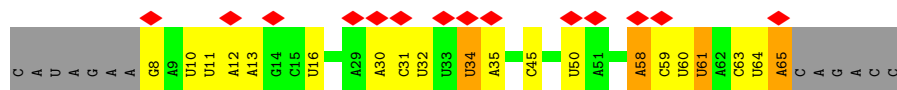
- Molecule 52: ulr14



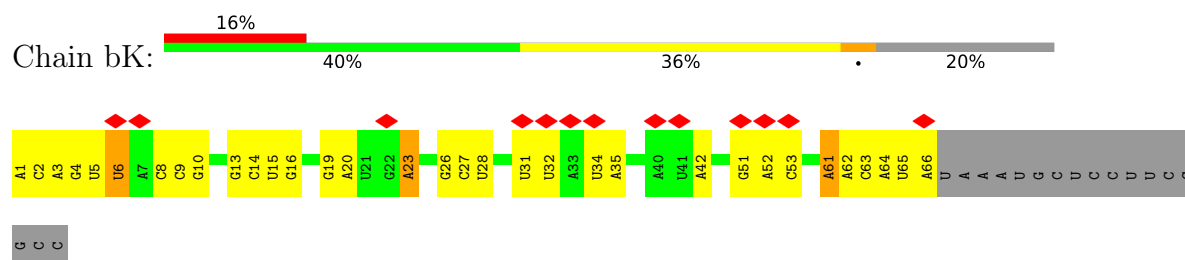
- Molecule 53: ulr15



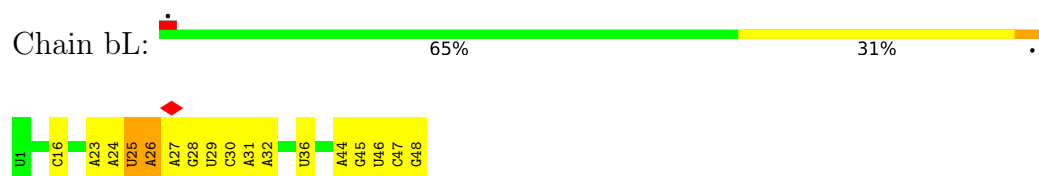
- Molecule 54: RNA33



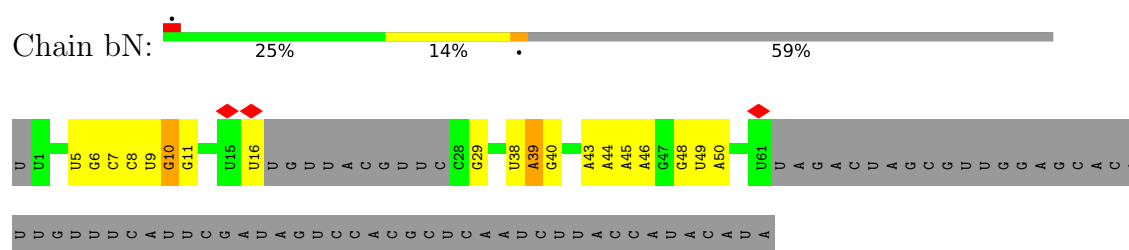
- Molecule 55: RNA5



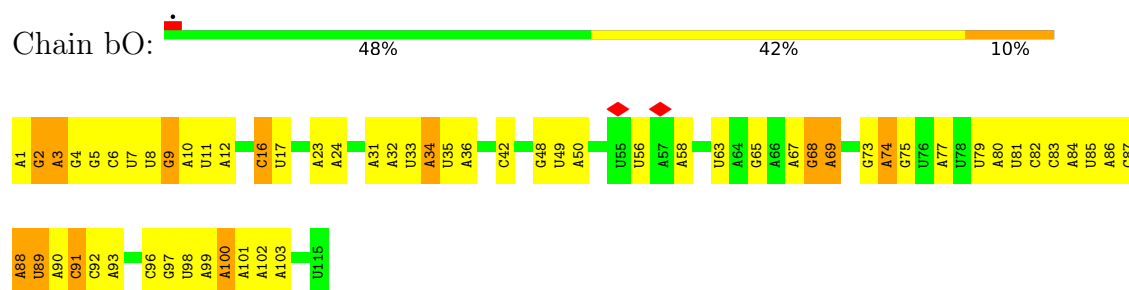
- Molecule 56: RNA17



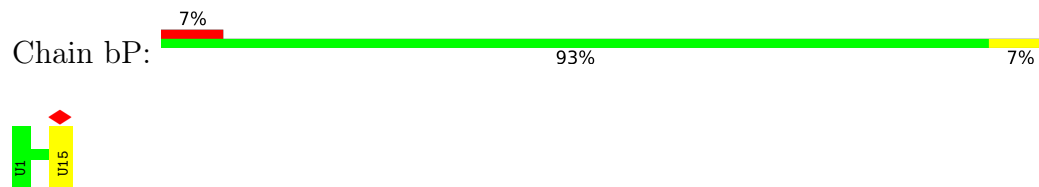
- Molecule 57: SSUB



- Molecule 58: SSUA



- Molecule 59: ulr16

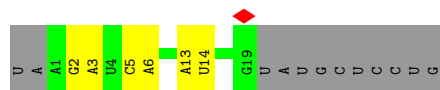


- Molecule 60: ulr17



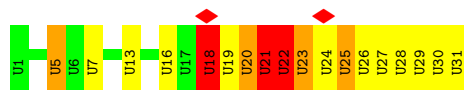
- Molecule 61: RNA30

Chain bR: 



- Molecule 62: url18

Chain bS: 




- Molecule 63: SSUF

Chain bT: 



- Molecule 64: ulr19

Chain bU: 



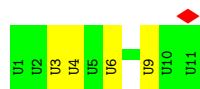
- Molecule 65: ulr20

Chain bV: 



- Molecule 66: ulr21

Chain bY: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	22169	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	59000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.159	Depositor
Minimum map value	-0.015	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	632.394, 632.394, 632.394	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.5057, 1.5057, 1.5057	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	B0	1.81	67/2369 (2.8%)	1.51	16/3204 (0.5%)
3	B2	1.19	23/2853 (0.8%)	1.13	14/3844 (0.4%)
4	B3	1.10	16/1767 (0.9%)	0.98	3/2381 (0.1%)
5	B4	0.56	0/682	0.60	1/914 (0.1%)
6	B5	0.30	0/1129	0.56	0/1513
7	B6	1.71	14/967 (1.4%)	1.52	7/1298 (0.5%)
10	B9	0.78	4/546 (0.7%)	0.68	2/730 (0.3%)
11	BA	0.74	2/4190 (0.0%)	0.71	4/5693 (0.1%)
12	BB	1.63	74/4388 (1.7%)	1.35	24/5925 (0.4%)
13	BC	0.81	11/1617 (0.7%)	0.75	7/2196 (0.3%)
14	BD	1.88	50/2738 (1.8%)	1.55	20/3720 (0.5%)
15	BE	1.35	41/5196 (0.8%)	1.26	23/7021 (0.3%)
16	BF	1.23	23/2259 (1.0%)	1.06	9/3058 (0.3%)
17	BG	0.40	0/1217	0.52	0/1657
18	BH	1.19	10/1015 (1.0%)	0.99	2/1365 (0.1%)
21	BK	0.87	6/1713 (0.4%)	0.87	3/2311 (0.1%)
22	BL	1.33	13/912 (1.4%)	1.22	3/1228 (0.2%)
23	BO	0.39	2/2206 (0.1%)	0.55	0/2975
25	BQ	1.24	32/3683 (0.9%)	1.06	6/5001 (0.1%)
26	BS	0.54	0/1334	0.67	0/1796
27	BT	1.60	11/830 (1.3%)	1.36	5/1131 (0.4%)
29	BV	0.57	3/2242 (0.1%)	0.63	2/3045 (0.1%)
30	BW	1.54	44/2773 (1.6%)	1.29	18/3752 (0.5%)
34	Bc	0.32	0/4386	0.49	0/5958
37	Bg	1.67	35/1602 (2.2%)	1.38	11/2164 (0.5%)
38	Bh	0.93	10/1272 (0.8%)	0.85	3/1710 (0.2%)
39	Bi	1.05	9/947 (1.0%)	0.94	4/1278 (0.3%)
40	Bk	1.06	13/3445 (0.4%)	1.00	5/4624 (0.1%)
41	Bl	0.94	19/1696 (1.1%)	0.85	3/2277 (0.1%)
42	HJ	1.31	45/2987 (1.5%)	1.16	15/4027 (0.4%)
43	HS	0.70	0/733	0.75	0/986
44	b1	1.07	0/175	1.31	0/268
45	b2	0.26	0/705	0.74	0/1094
46	b3	1.30	2/109 (1.8%)	1.52	4/166 (2.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
47	b4	2.73	56/655 (8.5%)	2.68	78/1021 (7.6%)
48	bA	0.35	0/636	0.79	0/988
49	bD	1.36	8/613 (1.3%)	1.55	20/956 (2.1%)
50	bE	0.26	0/2199	0.75	3/3425 (0.1%)
51	bG	1.05	1/87 (1.1%)	1.47	1/132 (0.8%)
52	bH	1.43	0/43	2.22	3/64 (4.7%)
53	bI	0.85	0/65	1.58	2/98 (2.0%)
54	bJ	0.66	3/1361 (0.2%)	1.24	21/2114 (1.0%)
55	bK	2.14	72/1562 (4.6%)	2.09	102/2428 (4.2%)
56	bL	1.59	32/1138 (2.8%)	1.68	47/1770 (2.7%)
57	bN	1.76	38/1194 (3.2%)	1.77	55/1857 (3.0%)
58	bO	2.27	143/2744 (5.2%)	2.19	202/4272 (4.7%)
59	bP	0.80	0/329	1.19	0/506
60	bQ	1.88	10/307 (3.3%)	1.43	0/472
61	bR	1.02	5/457 (1.1%)	1.26	9/710 (1.3%)
62	bS	1.13	0/681	1.97	32/1050 (3.0%)
63	bT	0.61	0/1267	1.12	13/1976 (0.7%)
64	bU	1.05	0/549	1.44	2/846 (0.2%)
65	bV	1.55	4/131 (3.1%)	1.51	3/200 (1.5%)
66	bY	1.19	2/241 (0.8%)	1.26	0/370
All	All	1.27	953/82942 (1.1%)	1.22	807/115565 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
15	BE	0	1
42	HJ	0	1
52	bH	0	1
62	bS	0	4
63	bT	0	2
All	All	0	9

All (953) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	BE	935	PRO	N-CD	-13.11	1.29	1.47
55	bK	3	A	C6-N6	-12.84	1.23	1.33
56	bL	27	A	C6-N6	-12.63	1.23	1.33
56	bL	26	A	C6-N6	-12.60	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	b4	5	A	C6-N6	-12.57	1.23	1.33
58	bO	88	A	C6-N6	-12.54	1.24	1.33
58	bO	90	A	C6-N6	-12.54	1.24	1.33
55	bK	61	A	C6-N6	-12.53	1.24	1.33
58	bO	102	A	C6-N6	-12.52	1.24	1.33
57	bN	43	A	C6-N6	-12.52	1.24	1.33
58	bO	32	A	C6-N6	-12.52	1.24	1.33
57	bN	45	A	C6-N6	-12.51	1.24	1.33
58	bO	101	A	C6-N6	-12.51	1.24	1.33
55	bK	62	A	C6-N6	-12.49	1.24	1.33
58	bO	100	A	C6-N6	-12.49	1.24	1.33
58	bO	84	A	C6-N6	-12.48	1.24	1.33
58	bO	1	A	C6-N6	-12.48	1.24	1.33
58	bO	99	A	C6-N6	-12.48	1.24	1.33
57	bN	44	A	C6-N6	-12.47	1.24	1.33
58	bO	58	A	C6-N6	-12.47	1.24	1.33
58	bO	3	A	C6-N6	-12.46	1.24	1.33
58	bO	31	A	C6-N6	-12.46	1.24	1.33
57	bN	46	A	C6-N6	-12.44	1.24	1.33
55	bK	1	A	C6-N6	-12.43	1.24	1.33
58	bO	50	A	C6-N6	-12.42	1.24	1.33
55	bK	64	A	C6-N6	-12.42	1.24	1.33
58	bO	74	A	C6-N6	-12.42	1.24	1.33
58	bO	93	A	C6-N6	-12.42	1.24	1.33
56	bL	23	A	C6-N6	-12.41	1.24	1.33
56	bL	24	A	C6-N6	-12.41	1.24	1.33
58	bO	10	A	C6-N6	-12.41	1.24	1.33
55	bK	20	A	C6-N6	-12.40	1.24	1.33
58	bO	69	A	C6-N6	-12.39	1.24	1.33
58	bO	34	A	C6-N6	-12.35	1.24	1.33
58	bO	80	A	C6-N6	-12.35	1.24	1.33
55	bK	66	A	C6-N6	-12.20	1.24	1.33
58	bO	6	C	C4-N4	-11.26	1.23	1.33
55	bK	27	C	C4-N4	-11.18	1.23	1.33
58	bO	87	C	C4-N4	-11.13	1.24	1.33
58	bO	16	C	C4-N4	-11.12	1.24	1.33
57	bN	8	C	C4-N4	-11.09	1.24	1.33
58	bO	82	C	C4-N4	-11.09	1.24	1.33
58	bO	96	C	C4-N4	-11.08	1.24	1.33
57	bN	7	C	C4-N4	-11.08	1.24	1.33
58	bO	83	C	C4-N4	-11.06	1.24	1.33
55	bK	63	C	C4-N4	-11.05	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	bO	91	C	C4-N4	-11.05	1.24	1.33
58	bO	92	C	C4-N4	-11.04	1.24	1.33
55	bK	14	C	C4-N4	-10.86	1.24	1.33
47	b4	13	C	C4-N4	-10.81	1.24	1.33
55	bK	2	C	C4-N4	-10.70	1.24	1.33
58	bO	9	G	C2-N2	-10.12	1.24	1.34
56	bL	44	A	C6-N6	-10.09	1.25	1.33
55	bK	16	G	C2-N2	-10.08	1.24	1.34
57	bN	11	G	C2-N2	-10.08	1.24	1.34
47	b4	4	G	C2-N2	-10.07	1.24	1.34
47	b4	23	A	C6-N6	-10.06	1.25	1.33
55	bK	13	G	C2-N2	-10.06	1.24	1.34
47	b4	3	G	C2-N2	-10.05	1.24	1.34
47	b4	18	A	C6-N6	-10.01	1.25	1.33
55	bK	4	G	C2-N2	-10.00	1.24	1.34
58	bO	68	G	C2-N2	-9.99	1.24	1.34
58	bO	5	G	C2-N2	-9.99	1.24	1.34
55	bK	19	G	C2-N2	-9.95	1.24	1.34
57	bN	10	G	C2-N2	-9.95	1.24	1.34
58	bO	2	G	C2-N2	-9.95	1.24	1.34
58	bO	48	G	C2-N2	-9.95	1.24	1.34
57	bN	6	G	C2-N2	-9.94	1.24	1.34
58	bO	6	C	C5-C6	-9.93	1.26	1.34
56	bL	47	C	C5-C6	-9.93	1.26	1.34
58	bO	73	G	C2-N2	-9.90	1.24	1.34
47	b4	12	G	C2-N2	-9.89	1.24	1.34
47	b4	17	G	C2-N2	-9.88	1.24	1.34
55	bK	26	G	C2-N2	-9.87	1.24	1.34
47	b4	16	G	C2-N2	-9.83	1.24	1.34
55	bK	27	C	C5-C6	-9.79	1.26	1.34
47	b4	25	C	C5-C6	-9.77	1.26	1.34
55	bK	2	C	C5-C6	-9.77	1.26	1.34
58	bO	4	G	C2-N2	-9.75	1.24	1.34
55	bK	63	C	C5-C6	-9.55	1.26	1.34
57	bN	8	C	C5-C6	-9.51	1.26	1.34
58	bO	92	C	C5-C6	-9.51	1.26	1.34
58	bO	87	C	C5-C6	-9.49	1.26	1.34
47	b4	13	C	C5-C6	-9.48	1.26	1.34
58	bO	91	C	C5-C6	-9.44	1.26	1.34
57	bN	7	C	C5-C6	-9.41	1.26	1.34
58	bO	83	C	C5-C6	-9.40	1.26	1.34
58	bO	82	C	C5-C6	-9.39	1.26	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	bO	96	C	C5-C6	-9.39	1.26	1.34
58	bO	16	C	C5-C6	-9.38	1.26	1.34
47	b4	7	G	C2-N2	-9.38	1.25	1.34
55	bK	14	C	C5-C6	-9.08	1.27	1.34
47	b4	25	C	C4-N4	-8.98	1.25	1.33
56	bL	47	C	C4-N4	-8.95	1.25	1.33
55	bK	15	U	C5-C6	-8.86	1.26	1.34
49	bD	26	A	C6-N6	-8.80	1.26	1.33
61	bR	3	A	C6-N6	-8.75	1.26	1.33
47	b4	21	U	C5-C6	-8.52	1.26	1.34
47	b4	27	U	C5-C6	-8.49	1.26	1.34
56	bL	46	U	C5-C6	-8.41	1.26	1.34
57	bN	9	U	C5-C6	-8.26	1.26	1.34
55	bK	28	U	C5-C6	-8.19	1.26	1.34
57	bN	5	U	C5-C6	-8.18	1.26	1.34
58	bO	98	U	C5-C6	-8.18	1.26	1.34
58	bO	7	U	C5-C6	-8.17	1.26	1.34
55	bK	5	U	C5-C6	-8.16	1.26	1.34
58	bO	8	U	C5-C6	-8.16	1.26	1.34
58	bO	33	U	C5-C6	-8.16	1.26	1.34
47	b4	8	U	C5-C6	-8.15	1.26	1.34
58	bO	79	U	C5-C6	-8.15	1.26	1.34
58	bO	89	U	C5-C6	-8.15	1.26	1.34
58	bO	81	U	C5-C6	-8.14	1.26	1.34
56	bL	25	U	C5-C6	-8.14	1.26	1.34
55	bK	6	U	C5-C6	-8.14	1.26	1.34
58	bO	17	U	C5-C6	-8.13	1.26	1.34
55	bK	65	U	C5-C6	-8.12	1.26	1.34
58	bO	35	U	C5-C6	-8.12	1.26	1.34
58	bO	49	U	C5-C6	-8.11	1.26	1.34
58	bO	85	U	C5-C6	-8.09	1.26	1.34
56	bL	48	G	C2-N2	-8.07	1.26	1.34
47	b4	26	G	C2-N2	-8.02	1.26	1.34
47	b4	20	G	C2-N2	-8.02	1.26	1.34
14	BD	199	ARG	CZ-NH2	-8.01	1.22	1.33
14	BD	458	ARG	CZ-NH2	-8.01	1.22	1.33
14	BD	391	ARG	CZ-NH2	-8.00	1.22	1.33
14	BD	257	ARG	CZ-NH2	-8.00	1.22	1.33
56	bL	45	G	C2-N2	-7.98	1.26	1.34
12	BB	282	ARG	CZ-NH2	-7.97	1.22	1.33
14	BD	387	ARG	CZ-NH2	-7.97	1.22	1.33
1	B0	34	ARG	CZ-NH2	-7.96	1.22	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B0	268	ARG	CZ-NH2	-7.96	1.22	1.33
42	HJ	759	ARG	CZ-NH2	-7.96	1.22	1.33
12	BB	230	ARG	CZ-NH2	-7.95	1.22	1.33
40	Bk	114	ARG	CZ-NH2	-7.95	1.22	1.33
14	BD	265	ARG	CZ-NH2	-7.95	1.22	1.33
42	HJ	639	ARG	CZ-NH2	-7.95	1.22	1.33
1	B0	42	ARG	CZ-NH2	-7.94	1.22	1.33
12	BB	670	ARG	CZ-NH2	-7.94	1.22	1.33
1	B0	273	ARG	CZ-NH2	-7.94	1.22	1.33
42	HJ	751	ARG	CZ-NH2	-7.94	1.22	1.33
14	BD	368	ARG	CZ-NH2	-7.93	1.22	1.33
14	BD	470	ARG	CZ-NH2	-7.93	1.22	1.33
30	BW	286	ARG	CZ-NH2	-7.93	1.22	1.33
15	BE	492	ARG	CZ-NH2	-7.92	1.22	1.33
14	BD	207	ARG	CZ-NH2	-7.92	1.22	1.33
18	BH	88	ARG	CZ-NH2	-7.92	1.22	1.33
25	BQ	410	ARG	CZ-NH2	-7.92	1.22	1.33
1	B0	271	ARG	CZ-NH2	-7.92	1.22	1.33
38	Bh	129	ARG	CZ-NH2	-7.92	1.22	1.33
42	HJ	705	ARG	CZ-NH2	-7.92	1.22	1.33
4	B3	12	ARG	CZ-NH2	-7.92	1.22	1.33
12	BB	160	ARG	CZ-NH2	-7.91	1.22	1.33
1	B0	150	ARG	CZ-NH2	-7.91	1.22	1.33
42	HJ	741	ARG	CZ-NH2	-7.91	1.22	1.33
25	BQ	411	ARG	CZ-NH2	-7.91	1.22	1.33
41	Bl	3	ARG	CZ-NH2	-7.91	1.22	1.33
41	Bl	90	ARG	CZ-NH2	-7.91	1.22	1.33
42	HJ	685	ARG	CZ-NH2	-7.91	1.22	1.33
18	BH	67	ARG	CZ-NH2	-7.91	1.22	1.33
30	BW	322	ARG	CZ-NH2	-7.90	1.22	1.33
18	BH	86	ARG	CZ-NH2	-7.89	1.22	1.33
42	HJ	730	ARG	CZ-NH2	-7.89	1.22	1.33
4	B3	13	ARG	CZ-NH2	-7.89	1.22	1.33
16	BF	21	ARG	CZ-NH2	-7.89	1.22	1.33
25	BQ	469	ARG	CZ-NH2	-7.89	1.22	1.33
18	BH	64	ARG	CZ-NH2	-7.89	1.22	1.33
37	Bg	170	ARG	CZ-NH2	-7.89	1.22	1.33
10	B9	59	ARG	CZ-NH2	-7.89	1.22	1.33
14	BD	320	ARG	CZ-NH2	-7.89	1.22	1.33
16	BF	271	ARG	CZ-NH2	-7.89	1.22	1.33
16	BF	274	ARG	CZ-NH2	-7.89	1.22	1.33
37	Bg	97	ARG	CZ-NH2	-7.89	1.22	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	BE	394	ARG	CZ-NH2	-7.88	1.22	1.33
37	Bg	162	ARG	CZ-NH2	-7.88	1.22	1.33
49	bD	22	U	C5-C6	-7.88	1.27	1.34
16	BF	254	ARG	CZ-NH2	-7.88	1.22	1.33
15	BE	475	ARG	CZ-NH2	-7.88	1.22	1.33
37	Bg	219	ARG	CZ-NH2	-7.88	1.22	1.33
42	HJ	760	ARG	CZ-NH2	-7.88	1.22	1.33
12	BB	1153	ARG	CZ-NH1	-7.88	1.22	1.33
1	B0	264	ARG	CZ-NH2	-7.87	1.22	1.33
13	BC	43	ARG	CZ-NH2	-7.87	1.22	1.33
37	Bg	186	ARG	CZ-NH2	-7.86	1.22	1.33
30	BW	279	ARG	CZ-NH2	-7.86	1.22	1.33
13	BC	42	ARG	CZ-NH2	-7.85	1.22	1.33
16	BF	250	ARG	CZ-NH2	-7.84	1.22	1.33
3	B2	134	ARG	CZ-NH2	-7.84	1.22	1.33
16	BF	33	ARG	CZ-NH2	-7.83	1.22	1.33
41	Bl	14	ARG	CZ-NH2	-7.83	1.22	1.33
16	BF	32	ARG	CZ-NH2	-7.82	1.22	1.33
30	BW	321	ARG	CZ-NH2	-7.82	1.22	1.33
1	B0	36	ARG	CZ-NH2	-7.82	1.22	1.33
12	BB	1125	ARG	CZ-NH2	-7.82	1.22	1.33
1	B0	43	ARG	CZ-NH2	-7.81	1.22	1.33
16	BF	259	ARG	CZ-NH2	-7.81	1.22	1.33
30	BW	324	ARG	CZ-NH2	-7.80	1.23	1.33
21	BK	89	ARG	CZ-NH2	-7.79	1.23	1.33
12	BB	1124	ARG	CZ-NH2	-7.78	1.23	1.33
1	B0	305	ARG	CZ-NH2	-7.77	1.23	1.33
30	BW	236	ARG	CZ-NH2	-7.77	1.23	1.33
12	BB	426	ARG	CZ-NH2	-7.75	1.23	1.33
15	BE	327	ARG	CZ-NH2	-7.74	1.23	1.33
14	BD	131	ARG	CZ-NH2	-7.72	1.23	1.33
12	BB	68	ARG	CZ-NH2	-7.70	1.23	1.33
25	BQ	204	ARG	CZ-NH2	-7.70	1.23	1.33
13	BC	203	ARG	CZ-NH2	-7.68	1.23	1.33
13	BC	208	ARG	CZ-NH2	-7.67	1.23	1.33
25	BQ	373	ARG	CZ-NH2	-7.65	1.23	1.33
25	BQ	366	ARG	CZ-NH2	-7.63	1.23	1.33
49	bD	21	U	C5-C6	-7.63	1.27	1.34
30	BW	320	ARG	CZ-NH2	-7.62	1.23	1.33
49	bD	20	U	C5-C6	-7.60	1.27	1.34
30	BW	315	ARG	CZ-NH2	-7.55	1.23	1.33
30	BW	336	ARG	CZ-NH2	-7.53	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	BW	147	ARG	CZ-NH2	-7.50	1.23	1.33
14	BD	93	ARG	CZ-NH2	-7.50	1.23	1.33
12	BB	230	ARG	CZ-NH1	-7.49	1.23	1.33
37	Bg	89	ARG	CZ-NH2	-7.48	1.23	1.33
58	bO	4	G	C8-N7	-7.47	1.26	1.30
12	BB	282	ARG	CZ-NH1	-7.47	1.23	1.33
1	B0	42	ARG	CZ-NH1	-7.45	1.23	1.33
37	Bg	176	ARG	CZ-NH2	-7.45	1.23	1.33
14	BD	391	ARG	CZ-NH1	-7.45	1.23	1.33
12	BB	32	ARG	CZ-NH2	-7.45	1.23	1.33
12	BB	61	ARG	CZ-NH2	-7.44	1.23	1.33
42	HJ	705	ARG	CZ-NH1	-7.44	1.23	1.33
25	BQ	411	ARG	CZ-NH1	-7.43	1.23	1.33
37	Bg	219	ARG	CZ-NH1	-7.43	1.23	1.33
14	BD	387	ARG	CZ-NH1	-7.43	1.23	1.33
18	BH	64	ARG	CZ-NH1	-7.43	1.23	1.33
14	BD	458	ARG	CZ-NH1	-7.42	1.23	1.33
4	B3	12	ARG	CZ-NH1	-7.42	1.23	1.33
14	BD	199	ARG	CZ-NH1	-7.42	1.23	1.33
12	BB	670	ARG	CZ-NH1	-7.41	1.23	1.33
25	BQ	410	ARG	CZ-NH1	-7.41	1.23	1.33
18	BH	86	ARG	CZ-NH1	-7.41	1.23	1.33
15	BE	394	ARG	CZ-NH1	-7.41	1.23	1.33
14	BD	265	ARG	CZ-NH1	-7.40	1.23	1.33
42	HJ	759	ARG	CZ-NH1	-7.40	1.23	1.33
13	BC	42	ARG	CZ-NH1	-7.40	1.23	1.33
14	BD	470	ARG	CZ-NH1	-7.40	1.23	1.33
30	BW	279	ARG	CZ-NH1	-7.40	1.23	1.33
25	BQ	469	ARG	CZ-NH1	-7.39	1.23	1.33
30	BW	321	ARG	CZ-NH1	-7.39	1.23	1.33
41	Bl	3	ARG	CZ-NH1	-7.39	1.23	1.33
12	BB	160	ARG	CZ-NH1	-7.39	1.23	1.33
41	Bl	14	ARG	CZ-NH1	-7.39	1.23	1.33
16	BF	21	ARG	CZ-NH1	-7.39	1.23	1.33
42	HJ	730	ARG	CZ-NH1	-7.39	1.23	1.33
1	B0	273	ARG	CZ-NH1	-7.39	1.23	1.33
1	B0	150	ARG	CZ-NH1	-7.39	1.23	1.33
42	HJ	751	ARG	CZ-NH1	-7.38	1.23	1.33
1	B0	271	ARG	CZ-NH1	-7.38	1.23	1.33
14	BD	257	ARG	CZ-NH1	-7.38	1.23	1.33
1	B0	268	ARG	CZ-NH1	-7.38	1.23	1.33
16	BF	33	ARG	CZ-NH1	-7.38	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B2	134	ARG	CZ-NH1	-7.38	1.23	1.33
15	BE	475	ARG	CZ-NH1	-7.38	1.23	1.33
15	BE	492	ARG	CZ-NH1	-7.38	1.23	1.33
18	BH	67	ARG	CZ-NH1	-7.38	1.23	1.33
38	Bh	129	ARG	CZ-NH1	-7.37	1.23	1.33
42	HJ	639	ARG	CZ-NH1	-7.37	1.23	1.33
4	B3	13	ARG	CZ-NH1	-7.37	1.23	1.33
21	BK	89	ARG	CZ-NH1	-7.37	1.23	1.33
42	HJ	760	ARG	CZ-NH1	-7.37	1.23	1.33
16	BF	254	ARG	CZ-NH1	-7.37	1.23	1.33
1	B0	305	ARG	CZ-NH1	-7.36	1.23	1.33
14	BD	320	ARG	CZ-NH1	-7.36	1.23	1.33
37	Bg	186	ARG	CZ-NH1	-7.36	1.23	1.33
10	B9	59	ARG	CZ-NH1	-7.36	1.23	1.33
30	BW	322	ARG	CZ-NH1	-7.36	1.23	1.33
42	HJ	685	ARG	CZ-NH1	-7.36	1.23	1.33
42	HJ	741	ARG	CZ-NH1	-7.36	1.23	1.33
16	BF	271	ARG	CZ-NH1	-7.35	1.23	1.33
14	BD	207	ARG	CZ-NH1	-7.35	1.23	1.33
37	Bg	170	ARG	CZ-NH1	-7.35	1.23	1.33
16	BF	32	ARG	CZ-NH1	-7.35	1.23	1.33
41	Bl	90	ARG	CZ-NH1	-7.35	1.23	1.33
46	b3	3	U	P-OP1	7.35	1.61	1.49
37	Bg	97	ARG	CZ-NH1	-7.35	1.23	1.33
37	Bg	162	ARG	CZ-NH1	-7.35	1.23	1.33
16	BF	259	ARG	CZ-NH1	-7.34	1.23	1.33
12	BB	1153	ARG	CZ-NH2	-7.34	1.23	1.33
65	bV	1	U	P-OP1	7.34	1.61	1.49
1	B0	34	ARG	CZ-NH1	-7.33	1.23	1.33
40	Bk	114	ARG	CZ-NH1	-7.33	1.23	1.33
14	BD	368	ARG	CZ-NH1	-7.33	1.23	1.33
18	BH	88	ARG	CZ-NH1	-7.33	1.23	1.33
16	BF	274	ARG	CZ-NH1	-7.33	1.23	1.33
1	B0	36	ARG	CZ-NH1	-7.32	1.23	1.33
46	b3	4	U	P-OP1	7.32	1.61	1.49
65	bV	6	U	P-OP1	7.32	1.61	1.49
13	BC	43	ARG	CZ-NH1	-7.31	1.23	1.33
16	BF	250	ARG	CZ-NH1	-7.31	1.23	1.33
1	B0	43	ARG	CZ-NH1	-7.29	1.23	1.33
30	BW	324	ARG	CZ-NH1	-7.29	1.23	1.33
27	BT	44	ARG	CZ-NH2	-7.29	1.23	1.33
30	BW	286	ARG	CZ-NH1	-7.28	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B0	264	ARG	CZ-NH1	-7.27	1.23	1.33
30	BW	236	ARG	CZ-NH1	-7.26	1.23	1.33
12	BB	426	ARG	CZ-NH1	-7.19	1.23	1.33
15	BE	327	ARG	CZ-NH1	-7.19	1.23	1.33
12	BB	68	ARG	CZ-NH1	-7.19	1.23	1.33
12	BB	1125	ARG	CZ-NH1	-7.18	1.23	1.33
14	BD	131	ARG	CZ-NH1	-7.18	1.23	1.33
12	BB	1124	ARG	CZ-NH1	-7.17	1.23	1.33
25	BQ	366	ARG	CZ-NH1	-7.16	1.23	1.33
25	BQ	204	ARG	CZ-NH1	-7.14	1.23	1.33
13	BC	203	ARG	CZ-NH1	-7.13	1.23	1.33
13	BC	208	ARG	CZ-NH1	-7.13	1.23	1.33
55	bK	66	A	C2'-C1'	-7.11	1.45	1.53
25	BQ	373	ARG	CZ-NH1	-7.10	1.23	1.33
30	BW	336	ARG	CZ-NH1	-7.07	1.23	1.33
30	BW	147	ARG	CZ-NH1	-7.05	1.23	1.33
61	bR	2	G	C2-N2	-7.05	1.27	1.34
58	bO	5	G	C8-N7	-7.03	1.26	1.30
30	BW	315	ARG	CZ-NH1	-7.01	1.24	1.33
49	bD	27	G	C2-N2	-7.00	1.27	1.34
30	BW	320	ARG	CZ-NH1	-6.99	1.24	1.33
37	Bg	89	ARG	CZ-NH1	-6.98	1.24	1.33
12	BB	61	ARG	CZ-NH1	-6.94	1.24	1.33
14	BD	93	ARG	CZ-NH1	-6.94	1.24	1.33
37	Bg	176	ARG	CZ-NH1	-6.94	1.24	1.33
15	BE	829	ARG	CZ-NH2	-6.91	1.24	1.33
47	b4	26	G	C8-N7	-6.91	1.26	1.30
55	bK	16	G	C8-N7	-6.88	1.26	1.30
15	BE	841	ARG	CZ-NH2	-6.87	1.24	1.33
12	BB	32	ARG	CZ-NH1	-6.86	1.24	1.33
47	b4	20	G	C8-N7	-6.86	1.26	1.30
47	b4	17	G	C8-N7	-6.83	1.26	1.30
57	bN	6	G	C8-N7	-6.83	1.26	1.30
56	bL	45	G	C8-N7	-6.83	1.26	1.30
58	bO	9	G	C8-N7	-6.82	1.26	1.30
55	bK	26	G	C8-N7	-6.80	1.26	1.30
54	bJ	8	G	C2-N2	-6.78	1.27	1.34
57	bN	10	G	C8-N7	-6.78	1.26	1.30
56	bL	48	G	C8-N7	-6.78	1.26	1.30
55	bK	4	G	C8-N7	-6.77	1.26	1.30
27	BT	44	ARG	CZ-NH1	-6.76	1.24	1.33
15	BE	765	ARG	CZ-NH2	-6.75	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	BE	560	ARG	CZ-NH2	-6.72	1.24	1.33
47	b4	3	G	C8-N7	-6.72	1.26	1.30
47	b4	4	G	C8-N7	-6.71	1.26	1.30
47	b4	16	G	C8-N7	-6.70	1.26	1.30
58	bO	2	G	C8-N7	-6.69	1.26	1.30
55	bK	13	G	C8-N7	-6.67	1.26	1.30
47	b4	12	G	C8-N7	-6.67	1.26	1.30
57	bN	11	G	C8-N7	-6.65	1.26	1.30
55	bK	19	G	C8-N7	-6.63	1.26	1.30
55	bK	2	C	C2'-C1'	-6.62	1.46	1.53
58	bO	73	G	C8-N7	-6.61	1.26	1.30
58	bO	68	G	C8-N7	-6.58	1.27	1.30
47	b4	7	G	C8-N7	-6.57	1.27	1.30
58	bO	48	G	C8-N7	-6.53	1.27	1.30
61	bR	2	G	C8-N7	-6.51	1.27	1.30
55	bK	66	A	C3'-C2'	-6.50	1.45	1.52
55	bK	2	C	N1-C6	-6.48	1.33	1.37
55	bK	2	C	C3'-C2'	-6.48	1.45	1.52
65	bV	6	U	C2'-C1'	-6.47	1.46	1.53
40	Bk	51	ARG	CZ-NH2	-6.43	1.24	1.33
27	BT	59	ARG	CZ-NH2	-6.43	1.24	1.33
40	Bk	34	ARG	CZ-NH2	-6.42	1.24	1.33
15	BE	829	ARG	CZ-NH1	-6.41	1.24	1.33
39	Bi	128	ARG	CZ-NH2	-6.40	1.24	1.33
15	BE	841	ARG	CZ-NH1	-6.40	1.24	1.33
27	BT	79	ARG	CZ-NH2	-6.40	1.24	1.33
40	Bk	30	ARG	CZ-NH2	-6.38	1.24	1.33
49	bD	27	G	C8-N7	-6.35	1.27	1.30
27	BT	62	ARG	CZ-NH2	-6.33	1.24	1.33
1	B0	171	ARG	CZ-NH2	-6.28	1.24	1.33
1	B0	242	ARG	CZ-NH2	-6.23	1.25	1.33
1	B0	249	ARG	CZ-NH2	-6.23	1.25	1.33
15	BE	560	ARG	CZ-NH1	-6.23	1.25	1.33
1	B0	165	ARG	CZ-NH2	-6.22	1.25	1.33
1	B0	181	ARG	CZ-NH2	-6.21	1.25	1.33
1	B0	294	ARG	CZ-NH2	-6.21	1.25	1.33
15	BE	765	ARG	CZ-NH1	-6.21	1.25	1.33
37	Bg	205	GLU	CD-OE2	-6.21	1.18	1.25
1	B0	241	ARG	CZ-NH2	-6.20	1.25	1.33
55	bK	16	G	N9-C8	-6.08	1.33	1.37
47	b4	25	C	N1-C6	-6.07	1.33	1.37
47	b4	18	A	C8-N7	-6.05	1.27	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	bO	4	G	N9-C8	-6.04	1.33	1.37
47	b4	20	G	N9-C8	-6.03	1.33	1.37
58	bO	87	C	N1-C6	-6.01	1.33	1.37
55	bK	27	C	N1-C6	-5.99	1.33	1.37
37	Bg	205	GLU	CD-OE1	-5.99	1.19	1.25
58	bO	5	G	N9-C8	-5.97	1.33	1.37
57	bN	6	G	N9-C8	-5.97	1.33	1.37
57	bN	8	C	N1-C6	-5.97	1.33	1.37
54	bJ	8	G	C8-N7	-5.95	1.27	1.30
42	HJ	604	ARG	CZ-NH2	-5.93	1.25	1.33
56	bL	47	C	N1-C6	-5.92	1.33	1.37
58	bO	96	C	N1-C6	-5.92	1.33	1.37
55	bK	3	A	C8-N7	-5.91	1.27	1.31
55	bK	1	A	C8-N7	-5.91	1.27	1.31
15	BE	845	ARG	CZ-NH2	-5.91	1.25	1.33
58	bO	92	C	N1-C6	-5.90	1.33	1.37
27	BT	62	ARG	CZ-NH1	-5.90	1.25	1.33
58	bO	16	C	N1-C6	-5.89	1.33	1.37
58	bO	83	C	N1-C6	-5.89	1.33	1.37
40	Bk	30	ARG	CZ-NH1	-5.89	1.25	1.33
65	bV	6	U	C3'-C2'	-5.89	1.46	1.52
56	bL	44	A	C8-N7	-5.88	1.27	1.31
58	bO	8	U	C5'-C4'	-5.88	1.44	1.51
40	Bk	34	ARG	CZ-NH1	-5.87	1.25	1.33
58	bO	11	U	C2'-O2'	-5.87	1.34	1.41
56	bL	45	G	N9-C8	-5.86	1.33	1.37
39	Bi	128	ARG	CZ-NH1	-5.86	1.25	1.33
47	b4	26	G	N9-C8	-5.85	1.33	1.37
27	BT	79	ARG	CZ-NH1	-5.84	1.25	1.33
7	B6	45	ARG	CZ-NH2	-5.84	1.25	1.33
40	Bk	51	ARG	CZ-NH1	-5.83	1.25	1.33
51	bG	2	U	C4-O4	-5.83	1.19	1.23
55	bK	4	G	N9-C8	-5.83	1.33	1.37
10	B9	61	GLY	N-CA	-5.83	1.37	1.46
47	b4	23	A	C8-N7	-5.83	1.27	1.31
58	bO	82	C	N1-C6	-5.83	1.33	1.37
56	bL	27	A	C8-N7	-5.82	1.27	1.31
47	b4	12	G	N9-C8	-5.82	1.33	1.37
27	BT	59	ARG	CZ-NH1	-5.81	1.25	1.33
7	B6	91	ARG	CZ-NH2	-5.80	1.25	1.33
23	BO	49	ARG	CZ-NH2	-5.80	1.25	1.33
7	B6	12	ARG	CZ-NH2	-5.80	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	bO	6	C	N1-C6	-5.80	1.33	1.37
40	Bk	236	ARG	CZ-NH2	-5.80	1.25	1.33
11	BA	129	ARG	CZ-NH2	-5.78	1.25	1.33
55	bK	63	C	N1-C6	-5.78	1.33	1.37
55	bK	13	G	N9-C8	-5.77	1.33	1.37
47	b4	5	A	C8-N7	-5.76	1.27	1.31
7	B6	63	ARG	CZ-NH2	-5.76	1.25	1.33
57	bN	45	A	C8-N7	-5.76	1.27	1.31
57	bN	7	C	N1-C6	-5.75	1.33	1.37
57	bN	11	G	N9-C8	-5.75	1.33	1.37
58	bO	91	C	N1-C6	-5.75	1.33	1.37
1	B0	249	ARG	CZ-NH1	-5.75	1.25	1.33
1	B0	294	ARG	CZ-NH1	-5.74	1.25	1.33
47	b4	16	G	N9-C8	-5.74	1.33	1.37
58	bO	101	A	C8-N7	-5.73	1.27	1.31
55	bK	19	G	N9-C8	-5.72	1.33	1.37
55	bK	26	G	N9-C8	-5.72	1.33	1.37
58	bO	100	A	C8-N7	-5.71	1.27	1.31
58	bO	84	A	C8-N7	-5.70	1.27	1.31
1	B0	181	ARG	CZ-NH1	-5.70	1.25	1.33
55	bK	64	A	C8-N7	-5.70	1.27	1.31
1	B0	241	ARG	CZ-NH1	-5.69	1.25	1.33
1	B0	242	ARG	CZ-NH1	-5.69	1.25	1.33
1	B0	165	ARG	CZ-NH1	-5.69	1.25	1.33
58	bO	80	A	C8-N7	-5.68	1.27	1.31
58	bO	98	U	C5'-C4'	-5.68	1.44	1.51
39	Bi	86	ARG	CZ-NH2	-5.68	1.25	1.33
47	b4	4	G	N9-C8	-5.68	1.33	1.37
56	bL	24	A	C8-N7	-5.68	1.27	1.31
58	bO	90	A	C8-N7	-5.68	1.27	1.31
47	b4	5	A	C5'-C4'	-5.67	1.44	1.51
25	BQ	506	ARG	CZ-NH2	-5.67	1.25	1.33
56	bL	26	A	C8-N7	-5.67	1.27	1.31
58	bO	10	A	C8-N7	-5.67	1.27	1.31
25	BQ	499	ARG	CZ-NH2	-5.67	1.25	1.33
30	BW	101	ARG	CZ-NH2	-5.67	1.25	1.33
47	b4	13	C	N1-C6	-5.67	1.33	1.37
58	bO	101	A	C5'-C4'	-5.67	1.44	1.51
56	bL	48	G	N9-C8	-5.66	1.33	1.37
58	bO	69	A	C8-N7	-5.66	1.27	1.31
58	bO	2	G	N9-C8	-5.66	1.33	1.37
22	BL	45	ARG	CZ-NH2	-5.66	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B0	171	ARG	CZ-NH1	-5.66	1.25	1.33
58	bO	9	G	N9-C8	-5.65	1.33	1.37
58	bO	7	U	C5'-C4'	-5.65	1.44	1.51
55	bK	14	C	N1-C6	-5.65	1.33	1.37
40	Bk	16	ARG	CZ-NH2	-5.65	1.25	1.33
57	bN	10	G	N9-C8	-5.65	1.33	1.37
58	bO	102	A	C8-N7	-5.65	1.27	1.31
55	bK	13	G	C5'-C4'	-5.64	1.44	1.51
39	Bi	124	TYR	CD2-CE2	-5.64	1.30	1.39
58	bO	58	A	C8-N7	-5.64	1.27	1.31
25	BQ	68	ARG	CZ-NH2	-5.64	1.25	1.33
57	bN	43	A	C8-N7	-5.64	1.27	1.31
4	B3	220	ARG	CZ-NH2	-5.63	1.25	1.33
58	bO	31	A	C8-N7	-5.63	1.27	1.31
58	bO	73	G	N9-C8	-5.63	1.33	1.37
60	bQ	9	U	C5'-C4'	-5.63	1.44	1.51
39	Bi	124	TYR	CD1-CE1	-5.63	1.30	1.39
47	b4	3	G	N9-C8	-5.63	1.33	1.37
58	bO	73	G	C5'-C4'	-5.63	1.44	1.51
18	BH	92	GLY	N-CA	-5.63	1.37	1.46
55	bK	66	A	N9-C8	-5.63	1.33	1.37
58	bO	50	A	C8-N7	-5.63	1.27	1.31
58	bO	32	A	C8-N7	-5.63	1.27	1.31
39	Bi	83	ARG	CZ-NH2	-5.63	1.25	1.33
58	bO	3	A	C8-N7	-5.63	1.27	1.31
27	BT	14	ARG	CZ-NH2	-5.62	1.25	1.33
47	b4	4	G	C5'-C4'	-5.62	1.44	1.51
66	bY	4	U	C5'-C4'	-5.62	1.44	1.51
55	bK	61	A	C8-N7	-5.62	1.27	1.31
56	bL	23	A	C8-N7	-5.62	1.27	1.31
22	BL	78	ARG	CZ-NH2	-5.62	1.25	1.33
55	bK	20	A	C5'-C4'	-5.62	1.44	1.51
58	bO	1	A	C8-N7	-5.62	1.27	1.31
22	BL	96	ARG	CZ-NH2	-5.61	1.25	1.33
55	bK	16	G	C5'-C4'	-5.60	1.44	1.51
58	bO	96	C	C5'-C4'	-5.60	1.44	1.51
55	bK	5	U	C5'-C4'	-5.60	1.44	1.51
57	bN	46	A	C5'-C4'	-5.60	1.44	1.51
55	bK	62	A	C8-N7	-5.59	1.27	1.31
60	bQ	4	U	C5'-C4'	-5.59	1.44	1.51
47	b4	16	G	C5'-C4'	-5.59	1.44	1.51
58	bO	85	U	C5'-C4'	-5.59	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B2	148	ARG	CZ-NH2	-5.59	1.25	1.33
4	B3	214	ARG	CZ-NH2	-5.59	1.25	1.33
47	b4	17	G	C5'-C4'	-5.59	1.44	1.51
55	bK	61	A	C5'-C4'	-5.59	1.44	1.51
57	bN	46	A	C8-N7	-5.59	1.27	1.31
3	B2	95	ARG	CZ-NH2	-5.58	1.25	1.33
58	bO	74	A	C8-N7	-5.58	1.27	1.31
58	bO	81	U	C5'-C4'	-5.58	1.44	1.51
58	bO	93	A	C8-N7	-5.58	1.27	1.31
57	bN	7	C	C5'-C4'	-5.58	1.44	1.51
58	bO	34	A	C8-N7	-5.58	1.27	1.31
66	bY	3	U	C5'-C4'	-5.58	1.44	1.51
1	B0	163	TYR	CD2-CE2	-5.58	1.30	1.39
22	BL	85	ARG	CZ-NH2	-5.58	1.25	1.33
55	bK	27	C	C5'-C4'	-5.58	1.44	1.51
58	bO	88	A	C8-N7	-5.57	1.27	1.31
4	B3	221	ARG	CZ-NH2	-5.57	1.25	1.33
1	B0	187	TYR	CD2-CE2	-5.57	1.30	1.39
3	B2	108	ARG	CZ-NH2	-5.57	1.25	1.33
47	b4	17	G	N9-C8	-5.57	1.33	1.37
4	B3	216	ARG	CZ-NH2	-5.57	1.25	1.33
3	B2	4	ARG	CZ-NH2	-5.57	1.25	1.33
15	BE	523	ARG	CZ-NH2	-5.57	1.25	1.33
55	bK	6	U	C5'-C4'	-5.57	1.44	1.51
57	bN	11	G	C5'-C4'	-5.57	1.44	1.51
55	bK	28	U	C5'-C4'	-5.56	1.44	1.51
58	bO	80	A	C5'-C4'	-5.56	1.44	1.51
42	HJ	710	GLY	N-CA	-5.56	1.37	1.46
57	bN	8	C	C5'-C4'	-5.56	1.44	1.51
57	bN	9	U	C5'-C4'	-5.55	1.44	1.51
58	bO	49	U	C5'-C4'	-5.55	1.44	1.51
57	bN	44	A	C5'-C4'	-5.55	1.44	1.51
58	bO	32	A	C5'-C4'	-5.54	1.44	1.51
60	bQ	12	U	C5'-C4'	-5.54	1.44	1.51
55	bK	19	G	C5'-C4'	-5.54	1.44	1.51
58	bO	99	A	C8-N7	-5.54	1.27	1.31
58	bO	48	G	N9-C8	-5.54	1.33	1.37
58	bO	87	C	C5'-C4'	-5.54	1.44	1.51
1	B0	163	TYR	CD1-CE1	-5.54	1.31	1.39
58	bO	79	U	C5'-C4'	-5.54	1.44	1.51
58	bO	92	C	C5'-C4'	-5.54	1.44	1.51
55	bK	64	A	C5'-C4'	-5.54	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	bO	33	U	C5'-C4'	-5.54	1.44	1.51
58	bO	83	C	C5'-C4'	-5.53	1.44	1.51
3	B2	46	ARG	CZ-NH2	-5.53	1.25	1.33
3	B2	91	ARG	CZ-NH2	-5.53	1.25	1.33
55	bK	62	A	C5'-C4'	-5.53	1.44	1.51
56	bL	24	A	C5'-C4'	-5.53	1.44	1.51
58	bO	68	G	N9-C8	-5.53	1.33	1.37
15	BE	534	ARG	CZ-NH2	-5.53	1.25	1.33
42	HJ	725	GLY	N-CA	-5.53	1.37	1.46
1	B0	187	TYR	CD1-CE1	-5.53	1.31	1.39
58	bO	31	A	C5'-C4'	-5.53	1.44	1.51
58	bO	100	A	C5'-C4'	-5.52	1.44	1.51
3	B2	145	ARG	CZ-NH2	-5.52	1.25	1.33
3	B2	133	ARG	CZ-NH2	-5.52	1.25	1.33
58	bO	50	A	C5'-C4'	-5.52	1.44	1.51
1	B0	70	GLY	N-CA	-5.52	1.37	1.46
47	b4	12	G	C5'-C4'	-5.52	1.44	1.51
58	bO	1	A	C5'-C4'	-5.52	1.44	1.51
41	Bl	91	GLY	N-CA	-5.52	1.37	1.46
55	bK	15	U	C5'-C4'	-5.52	1.44	1.51
58	bO	58	A	C5'-C4'	-5.52	1.44	1.51
47	b4	8	U	C5'-C4'	-5.51	1.44	1.51
55	bK	26	G	C5'-C4'	-5.51	1.44	1.51
16	BF	18	GLY	N-CA	-5.51	1.37	1.46
55	bK	20	A	C8-N7	-5.51	1.27	1.31
55	bK	66	A	C8-N7	-5.51	1.27	1.31
57	bN	10	G	C5'-C4'	-5.51	1.44	1.51
57	bN	45	A	C5'-C4'	-5.51	1.44	1.51
12	BB	948	ARG	CZ-NH2	-5.51	1.25	1.33
14	BD	211	TYR	CD1-CE1	-5.51	1.31	1.39
16	BF	248	TYR	CD2-CE2	-5.50	1.31	1.39
47	b4	13	C	C5'-C4'	-5.50	1.44	1.51
58	bO	89	U	C5'-C4'	-5.50	1.44	1.51
57	bN	44	A	C8-N7	-5.50	1.27	1.31
25	BQ	320	GLY	N-CA	-5.49	1.37	1.46
25	BQ	322	GLY	N-CA	-5.49	1.37	1.46
12	BB	172	TYR	CD1-CE1	-5.49	1.31	1.39
14	BD	17	ARG	CZ-NH2	-5.49	1.25	1.33
12	BB	172	TYR	CD2-CE2	-5.49	1.31	1.39
12	BB	1108	ARG	CZ-NH2	-5.48	1.25	1.33
55	bK	4	G	C5'-C4'	-5.48	1.44	1.51
1	B0	152	TYR	CD1-CE1	-5.48	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	b4	7	G	N9-C8	-5.48	1.34	1.37
12	BB	952	ARG	CZ-NH2	-5.48	1.25	1.33
47	b4	7	G	C5'-C4'	-5.48	1.44	1.51
14	BD	151	ARG	CZ-NH2	-5.48	1.25	1.33
42	HJ	604	ARG	CZ-NH1	-5.47	1.25	1.33
42	HJ	717	TYR	CD1-CE1	-5.47	1.31	1.39
13	BC	44	TYR	CD1-CE1	-5.47	1.31	1.39
58	bO	69	A	C5'-C4'	-5.47	1.44	1.51
13	BC	44	TYR	CD2-CE2	-5.47	1.31	1.39
55	bK	65	U	C5'-C4'	-5.47	1.44	1.51
21	BK	46	TYR	CD2-CE2	-5.46	1.31	1.39
58	bO	34	A	C5'-C4'	-5.46	1.44	1.51
58	bO	10	A	C5'-C4'	-5.46	1.44	1.51
1	B0	45	TYR	CD2-CE2	-5.46	1.31	1.39
37	Bg	58	ARG	CZ-NH2	-5.46	1.25	1.33
12	BB	1111	ARG	CZ-NH2	-5.46	1.25	1.33
14	BD	211	TYR	CD2-CE2	-5.46	1.31	1.39
58	bO	4	G	C5'-C4'	-5.46	1.44	1.51
14	BD	3	ARG	CZ-NH2	-5.46	1.25	1.33
1	B0	152	TYR	CD2-CE2	-5.45	1.31	1.39
58	bO	82	C	C5'-C4'	-5.45	1.44	1.51
42	HJ	734	TYR	CD2-CE2	-5.45	1.31	1.39
12	BB	947	ARG	CZ-NH2	-5.45	1.25	1.33
12	BB	981	ARG	CZ-NH2	-5.45	1.25	1.33
37	Bg	223	GLY	N-CA	-5.45	1.37	1.46
41	Bl	124	TYR	CD2-CE2	-5.45	1.31	1.39
60	bQ	2	U	C5'-C4'	-5.45	1.44	1.51
12	BB	280	GLY	N-CA	-5.45	1.37	1.46
12	BB	963	ARG	CZ-NH2	-5.45	1.25	1.33
58	bO	48	G	C5'-C4'	-5.45	1.44	1.51
15	BE	389	GLY	N-CA	-5.44	1.37	1.46
58	bO	84	A	C5'-C4'	-5.44	1.44	1.51
37	Bg	59	ARG	CZ-NH2	-5.44	1.25	1.33
58	bO	3	A	C5'-C4'	-5.44	1.44	1.51
12	BB	1007	ARG	CZ-NH2	-5.44	1.25	1.33
55	bK	63	C	C5'-C4'	-5.44	1.44	1.51
27	BT	48	GLY	N-CA	-5.43	1.38	1.46
57	bN	6	G	C5'-C4'	-5.43	1.44	1.51
12	BB	1112	ARG	CZ-NH2	-5.43	1.25	1.33
57	bN	43	A	C5'-C4'	-5.43	1.44	1.51
58	bO	17	U	C5'-C4'	-5.43	1.44	1.51
47	b4	3	G	C5'-C4'	-5.43	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	BW	141	GLY	N-CA	-5.43	1.38	1.46
42	HJ	722	TYR	CD1-CE1	-5.43	1.31	1.39
58	bO	5	G	C5'-C4'	-5.43	1.44	1.51
60	bQ	3	U	C5'-C4'	-5.43	1.44	1.51
16	BF	248	TYR	CD1-CE1	-5.42	1.31	1.39
60	bQ	13	U	C5'-C4'	-5.42	1.44	1.51
12	BB	1130	GLY	N-CA	-5.42	1.38	1.46
56	bL	23	A	C5'-C4'	-5.42	1.44	1.51
58	bO	93	A	C5'-C4'	-5.42	1.44	1.51
41	Bl	124	TYR	CD1-CE1	-5.42	1.31	1.39
1	B0	45	TYR	CD1-CE1	-5.41	1.31	1.39
38	Bh	131	TYR	CD2-CE2	-5.41	1.31	1.39
42	HJ	722	TYR	CD2-CE2	-5.41	1.31	1.39
37	Bg	80	TYR	CD2-CE2	-5.41	1.31	1.39
21	BK	46	TYR	CD1-CE1	-5.41	1.31	1.39
42	HJ	717	TYR	CD2-CE2	-5.41	1.31	1.39
61	bR	3	A	C8-N7	-5.41	1.27	1.31
29	BV	225	TYR	CD1-CE1	-5.41	1.31	1.39
57	bN	5	U	C5'-C4'	-5.40	1.44	1.51
4	B3	6	TYR	CD1-CE1	-5.40	1.31	1.39
38	Bh	131	TYR	CD1-CE1	-5.40	1.31	1.39
37	Bg	174	TYR	CD1-CE1	-5.39	1.31	1.39
1	B0	251	GLY	N-CA	-5.39	1.38	1.46
15	BE	832	GLY	N-CA	-5.39	1.38	1.46
61	bR	2	G	N9-C8	-5.39	1.34	1.37
12	BB	983	ARG	CZ-NH2	-5.38	1.26	1.33
29	BV	225	TYR	CD2-CE2	-5.38	1.31	1.39
4	B3	6	TYR	CD2-CE2	-5.38	1.31	1.39
12	BB	308	LYS	CE-NZ	-5.38	1.35	1.49
42	HJ	750	LYS	CE-NZ	-5.38	1.35	1.49
42	HJ	684	GLY	N-CA	-5.38	1.38	1.46
42	HJ	734	TYR	CD1-CE1	-5.38	1.31	1.39
37	Bg	90	GLY	N-CA	-5.37	1.38	1.46
40	Bk	38	GLY	N-CA	-5.36	1.38	1.46
58	bO	35	U	C5'-C4'	-5.36	1.45	1.51
58	bO	6	C	C4-C5	-5.36	1.38	1.43
30	BW	149	VAL	CB-CG2	-5.36	1.41	1.52
1	B0	153	GLY	N-CA	-5.35	1.38	1.46
15	BE	845	ARG	CZ-NH1	-5.35	1.26	1.33
37	Bg	10	GLY	N-CA	-5.35	1.38	1.46
55	bK	14	C	C5'-C4'	-5.35	1.45	1.51
12	BB	1151	GLY	N-CA	-5.34	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	BW	293	GLY	N-CA	-5.34	1.38	1.46
37	Bg	80	TYR	CD1-CE1	-5.34	1.31	1.39
60	bQ	6	U	C5'-C4'	-5.34	1.45	1.51
15	BE	409	GLY	N-CA	-5.34	1.38	1.46
38	Bh	150	VAL	CB-CG1	-5.34	1.41	1.52
39	Bi	88	TRP	CD1-NE1	-5.33	1.28	1.38
1	B0	139	LYS	CE-NZ	-5.33	1.35	1.49
12	BB	313	LYS	CE-NZ	-5.33	1.35	1.49
1	B0	67	SER	CB-OG	-5.33	1.35	1.42
25	BQ	277	GLY	N-CA	-5.32	1.38	1.46
58	bO	16	C	C5'-C4'	-5.32	1.45	1.51
1	B0	248	TRP	CD1-NE1	-5.32	1.28	1.38
37	Bg	174	TYR	CD2-CE2	-5.31	1.31	1.39
15	BE	483	GLY	N-CA	-5.31	1.38	1.46
58	bO	88	A	C5'-C4'	-5.31	1.45	1.51
38	Bh	139	VAL	CB-CG2	-5.30	1.41	1.52
14	BD	459	GLY	N-CA	-5.30	1.38	1.46
37	Bg	216	LYS	CE-NZ	-5.30	1.35	1.49
55	bK	1	A	C5'-C4'	-5.30	1.45	1.51
15	BE	512	SER	CB-OG	-5.30	1.35	1.42
58	bO	91	C	C5'-C4'	-5.30	1.45	1.51
1	B0	240	TRP	CD1-NE1	-5.30	1.28	1.38
14	BD	92	GLY	N-CA	-5.30	1.38	1.46
1	B0	35	GLY	N-CA	-5.29	1.38	1.46
30	BW	287	LYS	CE-NZ	-5.29	1.35	1.49
37	Bg	185	GLY	N-CA	-5.29	1.38	1.46
16	BF	257	SER	CB-OG	-5.29	1.35	1.42
42	HJ	842	TRP	CD1-NE1	-5.29	1.28	1.38
12	BB	60	LYS	CE-NZ	-5.29	1.35	1.49
16	BF	25	LYS	CE-NZ	-5.29	1.35	1.49
41	Bl	20	LYS	CE-NZ	-5.29	1.35	1.49
12	BB	70	VAL	CB-CG1	-5.29	1.41	1.52
37	Bg	220	LYS	CE-NZ	-5.28	1.35	1.49
12	BB	425	LYS	CE-NZ	-5.28	1.35	1.49
42	HJ	712	LYS	CE-NZ	-5.28	1.35	1.49
47	b4	18	A	N9-C8	-5.28	1.33	1.37
12	BB	427	VAL	CB-CG1	-5.28	1.41	1.52
42	HJ	709	LYS	CE-NZ	-5.28	1.35	1.49
1	B0	177	TRP	CD1-NE1	-5.27	1.28	1.38
41	Bl	123	LYS	CE-NZ	-5.27	1.35	1.49
12	BB	142	SER	CB-OG	-5.27	1.35	1.42
25	BQ	359	VAL	CB-CG2	-5.27	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	BB	1022	ARG	CZ-NH2	-5.27	1.26	1.33
1	B0	6	TRP	CD1-NE1	-5.27	1.28	1.38
12	BB	427	VAL	CB-CG2	-5.27	1.41	1.52
12	BB	302	GLY	N-CA	-5.27	1.38	1.46
41	Bl	103	LYS	CE-NZ	-5.27	1.35	1.49
58	bO	99	A	C5'-C4'	-5.27	1.45	1.51
12	BB	78	VAL	CB-CG2	-5.27	1.41	1.52
16	BF	270	LYS	CE-NZ	-5.27	1.35	1.49
1	B0	5	TRP	CD1-NE1	-5.26	1.29	1.38
37	Bg	93	SER	CB-OG	-5.26	1.35	1.42
42	HJ	703	VAL	CB-CG1	-5.26	1.41	1.52
42	HJ	703	VAL	CB-CG2	-5.26	1.41	1.52
1	B0	162	VAL	CB-CG1	-5.26	1.41	1.52
7	B6	63	ARG	CZ-NH1	-5.26	1.26	1.33
42	HJ	747	LYS	CE-NZ	-5.26	1.35	1.49
12	BB	70	VAL	CB-CG2	-5.26	1.41	1.52
14	BD	442	SER	CB-OG	-5.26	1.35	1.42
1	B0	151	SER	CB-OG	-5.26	1.35	1.42
7	B6	45	ARG	CZ-NH1	-5.26	1.26	1.33
30	BW	207	VAL	CB-CG2	-5.26	1.41	1.52
12	BB	137	SER	CB-OG	-5.25	1.35	1.42
7	B6	12	ARG	CZ-NH1	-5.25	1.26	1.33
14	BD	472	SER	CB-OG	-5.25	1.35	1.42
56	bL	45	G	C5'-C4'	-5.25	1.45	1.51
1	B0	59	SER	CB-OG	-5.25	1.35	1.42
15	BE	513	SER	CB-OG	-5.25	1.35	1.42
12	BB	306	VAL	CB-CG1	-5.25	1.41	1.52
42	HJ	732	SER	CB-OG	-5.25	1.35	1.42
11	BA	129	ARG	CZ-NH1	-5.25	1.26	1.33
14	BD	130	GLY	N-CA	-5.25	1.38	1.46
37	Bg	225	SER	CB-OG	-5.25	1.35	1.42
41	Bl	18	VAL	CB-CG1	-5.25	1.41	1.52
47	b4	26	G	C5'-C4'	-5.24	1.45	1.51
12	BB	283	VAL	CB-CG2	-5.24	1.41	1.52
25	BQ	359	VAL	CB-CG1	-5.24	1.41	1.52
37	Bg	183	VAL	CB-CG2	-5.24	1.41	1.52
12	BB	306	VAL	CB-CG2	-5.24	1.41	1.52
30	BW	206	GLY	N-CA	-5.24	1.38	1.46
14	BD	212	VAL	CB-CG1	-5.24	1.41	1.52
1	B0	44	VAL	CB-CG2	-5.24	1.41	1.52
37	Bg	161	GLY	N-CA	-5.24	1.38	1.46
47	b4	20	G	C5'-C4'	-5.24	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B6	106	TYR	CD2-CE2	-5.23	1.31	1.39
12	BB	265	VAL	CB-CG2	-5.23	1.41	1.52
49	bD	26	A	C8-N7	-5.23	1.27	1.31
60	bQ	1	U	C5'-C4'	-5.23	1.45	1.51
1	B0	260	VAL	CB-CG2	-5.23	1.41	1.52
12	BB	283	VAL	CB-CG1	-5.23	1.41	1.52
38	Bh	150	VAL	CB-CG2	-5.23	1.41	1.52
40	Bk	236	ARG	CZ-NH1	-5.23	1.26	1.33
1	B0	44	VAL	CB-CG1	-5.23	1.41	1.52
22	BL	84	TYR	CD1-CE1	-5.23	1.31	1.39
57	bN	48	G	C2-N2	-5.23	1.29	1.34
55	bK	3	A	C5'-C4'	-5.23	1.45	1.51
23	BO	49	ARG	CZ-NH1	-5.22	1.26	1.33
14	BD	39	GLY	N-CA	-5.22	1.38	1.46
37	Bg	183	VAL	CB-CG1	-5.22	1.41	1.52
42	HJ	622	SER	CB-OG	-5.22	1.35	1.42
42	HJ	683	VAL	CB-CG2	-5.22	1.41	1.52
7	B6	91	ARG	CZ-NH1	-5.22	1.26	1.33
15	BE	385	SER	CB-OG	-5.22	1.35	1.42
21	BK	82	SER	CB-OG	-5.22	1.35	1.42
41	Bl	4	SER	CB-OG	-5.22	1.35	1.42
42	HJ	740	ALA	CA-CB	-5.22	1.41	1.52
60	bQ	7	U	C5'-C4'	-5.22	1.45	1.51
12	BB	263	SER	CB-OG	-5.22	1.35	1.42
25	BQ	356	VAL	CB-CG1	-5.22	1.41	1.52
56	bL	44	A	C5'-C4'	-5.22	1.45	1.51
12	BB	78	VAL	CB-CG1	-5.21	1.42	1.52
15	BE	413	SER	CB-OG	-5.21	1.35	1.42
30	BW	201	SER	CB-OG	-5.21	1.35	1.42
41	Bl	1	SER	CB-OG	-5.21	1.35	1.42
56	bL	25	U	C5'-C4'	-5.21	1.45	1.51
56	bL	26	A	C5'-C4'	-5.21	1.45	1.51
7	B6	3	TYR	CD2-CE2	-5.21	1.31	1.39
56	bL	46	U	C5'-C4'	-5.21	1.45	1.51
38	Bh	138	VAL	CB-CG2	-5.21	1.42	1.52
14	BD	216	ARG	CZ-NH2	-5.21	1.26	1.33
25	BQ	205	GLY	N-CA	-5.21	1.38	1.46
14	BD	471	SER	CB-OG	-5.21	1.35	1.42
21	BK	52	SER	CB-OG	-5.21	1.35	1.42
30	BW	289	SER	CB-OG	-5.21	1.35	1.42
14	BD	98	SER	CB-OG	-5.20	1.35	1.42
14	BD	255	VAL	CB-CG2	-5.20	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	BW	233	TRP	CD1-NE1	-5.20	1.29	1.38
37	Bg	215	SER	CB-OG	-5.20	1.35	1.42
42	HJ	683	VAL	CB-CG1	-5.20	1.42	1.52
42	HJ	731	VAL	CB-CG1	-5.20	1.42	1.52
3	B2	297	TYR	CD1-CE1	-5.20	1.31	1.39
30	BW	237	SER	CB-OG	-5.20	1.35	1.42
41	Bl	92	GLY	N-CA	-5.20	1.38	1.46
42	HJ	731	VAL	CB-CG2	-5.20	1.42	1.52
25	BQ	356	VAL	CB-CG2	-5.19	1.42	1.52
58	bO	2	G	C5'-C4'	-5.19	1.45	1.51
12	BB	265	VAL	CB-CG1	-5.19	1.42	1.52
29	BV	222	SER	CB-OG	-5.19	1.35	1.42
38	Bh	139	VAL	CB-CG1	-5.19	1.42	1.52
37	Bg	92	SER	CB-OG	-5.19	1.35	1.42
58	bO	9	G	C5'-C4'	-5.19	1.45	1.51
15	BE	515	SER	CB-OG	-5.19	1.35	1.42
14	BD	255	VAL	CB-CG1	-5.19	1.42	1.52
12	BB	267	GLY	N-CA	-5.18	1.38	1.46
58	bO	74	A	C5'-C4'	-5.18	1.45	1.51
30	BW	257	VAL	CB-CG2	-5.18	1.42	1.52
42	HJ	758	SER	CB-OG	-5.18	1.35	1.42
58	bO	90	A	C5'-C4'	-5.18	1.45	1.51
7	B6	3	TYR	CD1-CE1	-5.18	1.31	1.39
1	B0	261	VAL	CB-CG1	-5.18	1.42	1.52
47	b4	23	A	C5'-C4'	-5.18	1.45	1.51
14	BD	34	SER	CB-OG	-5.17	1.35	1.42
14	BD	212	VAL	CB-CG2	-5.17	1.42	1.52
1	B0	162	VAL	CB-CG2	-5.17	1.42	1.52
12	BB	336	SER	CB-OG	-5.17	1.35	1.42
15	BE	476	VAL	CB-CG2	-5.17	1.42	1.52
7	B6	106	TYR	CD1-CE1	-5.17	1.31	1.39
22	BL	92	TYR	CD2-CE2	-5.17	1.31	1.39
30	BW	333	GLY	N-CA	-5.17	1.38	1.46
12	BB	262	VAL	CB-CG1	-5.16	1.42	1.52
14	BD	440	SER	CB-OG	-5.16	1.35	1.42
22	BL	84	TYR	CD2-CE2	-5.16	1.31	1.39
14	BD	366	TRP	CD1-NE1	-5.16	1.29	1.38
47	b4	21	U	C5'-C4'	-5.16	1.45	1.51
14	BD	136	TRP	CD1-NE1	-5.16	1.29	1.38
30	BW	207	VAL	CB-CG1	-5.16	1.42	1.52
58	bO	6	C	C5'-C4'	-5.16	1.45	1.51
12	BB	146	TRP	CD1-NE1	-5.16	1.29	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	BB	1126	LYS	CE-NZ	-5.16	1.36	1.49
3	B2	297	TYR	CD2-CE2	-5.16	1.31	1.39
13	BC	68	SER	CB-OG	-5.16	1.35	1.42
15	BE	532	TRP	CD1-NE1	-5.16	1.29	1.38
22	BL	87	GLY	N-CA	-5.16	1.38	1.46
56	bL	44	A	N9-C8	-5.16	1.33	1.37
15	BE	480	TRP	CD1-NE1	-5.15	1.29	1.38
56	bL	47	C	C5'-C4'	-5.15	1.45	1.51
18	BH	94	TRP	CD1-NE1	-5.15	1.29	1.38
30	BW	323	TRP	CD1-NE1	-5.15	1.29	1.38
12	BB	442	TRP	CD1-NE1	-5.14	1.29	1.38
3	B2	264	TYR	CD2-CE2	-5.14	1.31	1.39
7	B6	66	TYR	CD1-CE1	-5.14	1.31	1.39
12	BB	148	VAL	CB-CG1	-5.14	1.42	1.52
38	Bh	138	VAL	CB-CG1	-5.14	1.42	1.52
42	HJ	742	TRP	CD1-NE1	-5.14	1.29	1.38
56	bL	27	A	C5'-C4'	-5.14	1.45	1.51
1	B0	261	VAL	CB-CG2	-5.14	1.42	1.52
22	BL	85	ARG	CZ-NH1	-5.14	1.26	1.33
27	BT	14	ARG	CZ-NH1	-5.14	1.26	1.33
58	bO	68	G	C5'-C4'	-5.14	1.45	1.51
1	B0	260	VAL	CB-CG1	-5.14	1.42	1.52
30	BW	314	SER	CB-OG	-5.14	1.35	1.42
39	Bi	86	ARG	CZ-NH1	-5.14	1.26	1.33
3	B2	264	TYR	CD1-CE1	-5.14	1.31	1.39
7	B6	66	TYR	CD2-CE2	-5.13	1.31	1.39
54	bJ	8	G	N9-C8	-5.13	1.34	1.37
1	B0	61	TRP	CD1-NE1	-5.13	1.29	1.38
30	BW	144	SER	CB-OG	-5.13	1.35	1.42
47	b4	18	A	C5'-C4'	-5.13	1.45	1.51
14	BD	202	TRP	CD1-NE1	-5.13	1.29	1.38
15	BE	382	VAL	CB-CG1	-5.13	1.42	1.52
15	BE	476	VAL	CB-CG1	-5.13	1.42	1.52
41	Bl	18	VAL	CB-CG2	-5.13	1.42	1.52
47	b4	25	C	C5'-C4'	-5.13	1.45	1.51
25	BQ	348	SER	CB-OG	-5.12	1.35	1.42
12	BB	30	SER	CB-OG	-5.12	1.35	1.42
16	BF	263	TRP	CD1-NE1	-5.12	1.29	1.38
30	BW	149	VAL	CB-CG1	-5.12	1.42	1.52
30	BW	292	GLY	N-CA	-5.12	1.38	1.46
10	B9	62	ALA	CA-CB	-5.12	1.41	1.52
15	BE	408	LYS	CE-NZ	-5.12	1.36	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BQ	68	ARG	CZ-NH1	-5.12	1.26	1.33
40	Bk	16	ARG	CZ-NH1	-5.12	1.26	1.33
4	B3	8	GLY	N-CA	-5.12	1.38	1.46
49	bD	27	G	N9-C8	-5.12	1.34	1.37
4	B3	14	VAL	CB-CG2	-5.11	1.42	1.52
22	BL	92	TYR	CD1-CE1	-5.11	1.31	1.39
22	BL	96	ARG	CZ-NH1	-5.11	1.26	1.33
39	Bi	83	ARG	CZ-NH1	-5.11	1.26	1.33
56	bL	48	G	C5'-C4'	-5.11	1.45	1.51
42	HJ	652	GLY	N-CA	-5.11	1.38	1.46
12	BB	262	VAL	CB-CG2	-5.11	1.42	1.52
14	BD	35	GLY	N-CA	-5.11	1.38	1.46
25	BQ	437	VAL	CB-CG1	-5.11	1.42	1.52
12	BB	148	VAL	CB-CG2	-5.11	1.42	1.52
15	BE	331	VAL	CB-CG1	-5.10	1.42	1.52
15	BE	407	TRP	CD1-NE1	-5.10	1.29	1.38
47	b4	23	A	N9-C8	-5.10	1.33	1.37
55	bK	3	A	N9-C8	-5.10	1.33	1.37
22	BL	78	ARG	CZ-NH1	-5.10	1.26	1.33
58	bO	102	A	C5'-C4'	-5.10	1.45	1.51
60	bQ	8	U	C5'-C4'	-5.10	1.45	1.51
30	BW	101	ARG	CZ-NH1	-5.10	1.26	1.33
42	HJ	649	GLY	N-CA	-5.10	1.38	1.46
1	B0	307	ALA	CA-CB	-5.09	1.41	1.52
22	BL	45	ARG	CZ-NH1	-5.09	1.26	1.33
1	B0	146	TRP	CD1-NE1	-5.09	1.29	1.38
4	B3	14	VAL	CB-CG1	-5.09	1.42	1.52
30	BW	326	GLY	N-CA	-5.09	1.38	1.46
3	B2	123	TYR	CD1-CE1	-5.09	1.31	1.39
3	B2	133	ARG	CZ-NH1	-5.09	1.26	1.33
30	BW	150	VAL	CB-CG1	-5.09	1.42	1.52
41	Bl	105	VAL	CB-CG2	-5.09	1.42	1.52
15	BE	382	VAL	CB-CG2	-5.09	1.42	1.52
30	BW	257	VAL	CB-CG1	-5.08	1.42	1.52
3	B2	91	ARG	CZ-NH1	-5.08	1.26	1.33
12	BB	33	SER	CB-OG	-5.07	1.35	1.42
25	BQ	506	ARG	CZ-NH1	-5.06	1.26	1.33
58	bO	58	A	N9-C8	-5.06	1.33	1.37
4	B3	221	ARG	CZ-NH1	-5.06	1.26	1.33
12	BB	63	GLY	N-CA	-5.06	1.38	1.46
12	BB	1128	TRP	CD1-NE1	-5.06	1.29	1.38
25	BQ	437	VAL	CB-CG2	-5.06	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	BE	523	ARG	CZ-NH1	-5.05	1.26	1.33
3	B2	4	ARG	CZ-NH1	-5.05	1.26	1.33
1	B0	66	ALA	CA-CB	-5.05	1.41	1.52
12	BB	31	TRP	CD1-NE1	-5.05	1.29	1.38
41	B1	105	VAL	CB-CG1	-5.05	1.42	1.52
58	bO	10	A	N9-C8	-5.05	1.33	1.37
3	B2	95	ARG	CZ-NH1	-5.05	1.26	1.33
14	BD	323	VAL	CB-CG2	-5.05	1.42	1.52
25	BQ	499	ARG	CZ-NH1	-5.04	1.26	1.33
3	B2	108	ARG	CZ-NH1	-5.04	1.26	1.33
12	BB	65	SER	CB-OG	-5.04	1.35	1.42
3	B2	123	TYR	CD2-CE2	-5.04	1.31	1.39
3	B2	148	ARG	CZ-NH1	-5.04	1.26	1.33
4	B3	220	ARG	CZ-NH1	-5.04	1.26	1.33
55	bK	27	C	C4-C5	-5.04	1.39	1.43
30	BW	150	VAL	CB-CG2	-5.03	1.42	1.52
3	B2	46	ARG	CZ-NH1	-5.02	1.26	1.33
25	BQ	138	GLY	N-CA	-5.02	1.38	1.46
12	BB	1115	TYR	CD1-CE1	-5.02	1.31	1.39
4	B3	216	ARG	CZ-NH1	-5.01	1.26	1.33
14	BD	323	VAL	CB-CG1	-5.01	1.42	1.52
15	BE	534	ARG	CZ-NH1	-5.01	1.26	1.33
25	BQ	278	VAL	CB-CG2	-5.00	1.42	1.52
57	bN	45	A	N9-C8	-5.00	1.33	1.37
25	BQ	350	VAL	CB-CG1	-5.00	1.42	1.52

All (807) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	bJ	63	C	O4'-C1'-N1	22.53	126.22	108.20
54	bJ	64	U	O4'-C1'-N1	13.24	118.79	108.20
58	bO	4	G	N7-C8-N9	12.30	119.25	113.10
55	bK	16	G	N7-C8-N9	12.24	119.22	113.10
47	b4	18	A	N1-C2-N3	12.23	135.41	129.30
56	bL	44	A	N1-C2-N3	12.20	135.40	129.30
47	b4	23	A	N1-C2-N3	12.19	135.40	129.30
58	bO	5	G	N7-C8-N9	12.12	119.16	113.10
47	b4	5	A	N1-C2-N3	12.04	135.32	129.30
47	b4	18	A	N7-C8-N9	12.02	119.81	113.80
62	bS	18	U	O4'-C1'-N1	11.97	117.78	108.20
57	bN	10	G	N7-C8-N9	11.96	119.08	113.10
56	bL	48	G	N7-C8-N9	11.90	119.05	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	bN	46	A	N1-C2-N3	11.88	135.24	129.30
55	bK	1	A	N7-C8-N9	11.88	119.74	113.80
57	bN	6	G	N7-C8-N9	11.86	119.03	113.10
55	bK	64	A	N1-C2-N3	11.85	135.23	129.30
55	bK	61	A	N1-C2-N3	11.79	135.20	129.30
47	b4	26	G	N7-C8-N9	11.78	118.99	113.10
58	bO	9	G	N7-C8-N9	11.78	118.99	113.10
56	bL	24	A	N1-C2-N3	11.77	135.19	129.30
58	bO	84	A	N1-C2-N3	11.77	135.18	129.30
57	bN	45	A	N1-C2-N3	11.76	135.18	129.30
58	bO	99	A	N1-C2-N3	11.76	135.18	129.30
58	bO	88	A	N1-C2-N3	11.76	135.18	129.30
58	bO	74	A	N1-C2-N3	11.75	135.18	129.30
58	bO	31	A	N1-C2-N3	11.75	135.17	129.30
58	bO	1	A	N1-C2-N3	11.74	135.17	129.30
55	bK	20	A	N1-C2-N3	11.73	135.16	129.30
58	bO	80	A	N1-C2-N3	11.71	135.16	129.30
58	bO	69	A	N1-C2-N3	11.70	135.15	129.30
58	bO	100	A	N1-C2-N3	11.70	135.15	129.30
58	bO	50	A	N1-C2-N3	11.69	135.15	129.30
58	bO	90	A	N1-C2-N3	11.69	135.15	129.30
55	bK	1	A	N1-C2-N3	11.69	135.14	129.30
58	bO	101	A	N1-C2-N3	11.68	135.14	129.30
56	bL	23	A	N1-C2-N3	11.66	135.13	129.30
55	bK	26	G	N7-C8-N9	11.65	118.93	113.10
55	bK	62	A	N1-C2-N3	11.65	135.13	129.30
56	bL	26	A	N1-C2-N3	11.65	135.12	129.30
58	bO	93	A	N1-C2-N3	11.65	135.12	129.30
56	bL	45	G	N7-C8-N9	11.64	118.92	113.10
58	bO	10	A	N1-C2-N3	11.63	135.12	129.30
57	bN	43	A	N1-C2-N3	11.62	135.11	129.30
47	b4	20	G	N7-C8-N9	11.61	118.91	113.10
58	bO	3	A	N1-C2-N3	11.61	135.11	129.30
58	bO	58	A	N1-C2-N3	11.61	135.10	129.30
55	bK	3	A	N1-C2-N3	11.61	135.10	129.30
55	bK	13	G	N7-C8-N9	11.60	118.90	113.10
58	bO	34	A	N1-C2-N3	11.57	135.09	129.30
58	bO	102	A	N1-C2-N3	11.57	135.08	129.30
58	bO	32	A	N1-C2-N3	11.56	135.08	129.30
56	bL	27	A	N1-C2-N3	11.54	135.07	129.30
47	b4	17	G	N7-C8-N9	11.51	118.85	113.10
57	bN	44	A	N1-C2-N3	11.48	135.04	129.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	bL	44	A	N7-C8-N9	11.47	119.54	113.80
47	b4	23	A	N7-C8-N9	11.41	119.50	113.80
47	b4	4	G	N7-C8-N9	11.34	118.77	113.10
55	bK	66	A	N1-C2-N3	11.31	134.96	129.30
57	bN	45	A	N7-C8-N9	11.29	119.45	113.80
47	b4	5	A	N7-C8-N9	11.26	119.43	113.80
47	b4	12	G	N7-C8-N9	11.24	118.72	113.10
58	bO	80	A	N7-C8-N9	11.24	119.42	113.80
56	bL	27	A	N7-C8-N9	11.24	119.42	113.80
47	b4	16	G	N7-C8-N9	11.22	118.71	113.10
58	bO	2	G	N7-C8-N9	11.22	118.71	113.10
47	b4	3	G	N7-C8-N9	11.22	118.71	113.10
58	bO	68	G	N7-C8-N9	11.21	118.71	113.10
55	bK	19	G	N7-C8-N9	11.21	118.70	113.10
58	bO	34	A	N7-C8-N9	11.18	119.39	113.80
58	bO	10	A	N7-C8-N9	11.18	119.39	113.80
58	bO	73	G	N7-C8-N9	11.18	118.69	113.10
56	bL	24	A	N7-C8-N9	11.17	119.39	113.80
58	bO	48	G	N7-C8-N9	11.15	118.67	113.10
55	bK	61	A	N7-C8-N9	11.14	119.37	113.80
58	bO	88	A	N7-C8-N9	11.14	119.37	113.80
55	bK	64	A	N7-C8-N9	11.13	119.37	113.80
47	b4	7	G	N7-C8-N9	11.12	118.66	113.10
61	bR	3	A	N1-C2-N3	11.12	134.86	129.30
57	bN	43	A	N7-C8-N9	11.12	119.36	113.80
57	bN	11	G	N7-C8-N9	11.11	118.66	113.10
56	bL	23	A	N7-C8-N9	11.10	119.35	113.80
55	bK	66	A	N7-C8-N9	11.07	119.34	113.80
55	bK	4	G	N7-C8-N9	11.07	118.64	113.10
58	bO	90	A	N7-C8-N9	11.07	119.33	113.80
58	bO	84	A	N7-C8-N9	11.06	119.33	113.80
58	bO	102	A	N7-C8-N9	11.05	119.32	113.80
55	bK	3	A	N7-C8-N9	11.03	119.31	113.80
58	bO	101	A	N7-C8-N9	11.01	119.31	113.80
58	bO	31	A	N7-C8-N9	11.00	119.30	113.80
58	bO	50	A	N7-C8-N9	11.00	119.30	113.80
58	bO	58	A	N7-C8-N9	11.00	119.30	113.80
58	bO	1	A	N7-C8-N9	11.00	119.30	113.80
49	bD	26	A	N1-C2-N3	10.99	134.80	129.30
58	bO	100	A	N7-C8-N9	10.96	119.28	113.80
55	bK	62	A	N7-C8-N9	10.96	119.28	113.80
58	bO	69	A	N7-C8-N9	10.96	119.28	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	bO	32	A	N7-C8-N9	10.95	119.27	113.80
58	bO	93	A	N7-C8-N9	10.94	119.27	113.80
58	bO	74	A	N7-C8-N9	10.94	119.27	113.80
55	bK	20	A	N7-C8-N9	10.94	119.27	113.80
57	bN	46	A	N7-C8-N9	10.94	119.27	113.80
63	bT	52	A	N1-C6-N6	-10.92	112.05	118.60
56	bL	26	A	N7-C8-N9	10.91	119.25	113.80
58	bO	3	A	N7-C8-N9	10.89	119.25	113.80
54	bJ	61	U	O4'-C1'-N1	10.88	116.90	108.20
58	bO	99	A	N7-C8-N9	10.86	119.23	113.80
57	bN	44	A	N7-C8-N9	10.79	119.20	113.80
61	bR	2	G	N7-C8-N9	10.78	118.49	113.10
49	bD	27	G	N7-C8-N9	10.68	118.44	113.10
61	bR	3	A	N7-C8-N9	10.62	119.11	113.80
49	bD	26	A	N7-C8-N9	10.28	118.94	113.80
47	b4	27	U	C2-N3-C4	9.97	132.98	127.00
56	bL	46	U	C2-N3-C4	9.96	132.98	127.00
54	bJ	65	A	N1-C6-N6	-9.96	112.63	118.60
54	bJ	8	G	N7-C8-N9	9.93	118.07	113.10
47	b4	21	U	C2-N3-C4	9.87	132.92	127.00
56	bL	45	G	C6-N1-C2	9.80	130.98	125.10
57	bN	9	U	C2-N3-C4	9.77	132.86	127.00
58	bO	89	U	C2-N3-C4	9.77	132.86	127.00
47	b4	20	G	C6-N1-C2	9.77	130.96	125.10
56	bL	48	G	C6-N1-C2	9.76	130.95	125.10
57	bN	5	U	C2-N3-C4	9.75	132.85	127.00
58	bO	79	U	C2-N3-C4	9.74	132.84	127.00
47	b4	8	U	C2-N3-C4	9.72	132.83	127.00
58	bO	85	U	C2-N3-C4	9.70	132.82	127.00
47	b4	26	G	C6-N1-C2	9.69	130.91	125.10
55	bK	65	U	C2-N3-C4	9.66	132.80	127.00
58	bO	17	U	C2-N3-C4	9.66	132.80	127.00
58	bO	49	U	C2-N3-C4	9.65	132.79	127.00
58	bO	8	U	C2-N3-C4	9.64	132.79	127.00
55	bK	16	G	C6-N1-C2	9.62	130.88	125.10
58	bO	81	U	C2-N3-C4	9.60	132.76	127.00
55	bK	14	C	C6-N1-C2	-9.57	116.47	120.30
55	bK	28	U	C2-N3-C4	9.56	132.74	127.00
58	bO	98	U	C2-N3-C4	9.56	132.73	127.00
55	bK	6	U	C2-N3-C4	9.55	132.73	127.00
58	bO	33	U	C2-N3-C4	9.53	132.72	127.00
58	bO	35	U	C2-N3-C4	9.52	132.71	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	bD	21	U	C2-N3-C4	9.51	132.71	127.00
55	bK	5	U	C2-N3-C4	9.51	132.70	127.00
58	bO	7	U	C2-N3-C4	9.50	132.70	127.00
47	b4	16	G	C6-N1-C2	9.46	130.78	125.10
47	b4	3	G	C6-N1-C2	9.45	130.77	125.10
56	bL	25	U	C2-N3-C4	9.45	132.67	127.00
47	b4	4	G	C6-N1-C2	9.44	130.77	125.10
47	b4	12	G	C6-N1-C2	9.44	130.77	125.10
57	bN	11	G	C6-N1-C2	9.43	130.76	125.10
58	bO	2	G	C6-N1-C2	9.41	130.75	125.10
47	b4	17	G	C6-N1-C2	9.41	130.74	125.10
57	bN	6	G	C6-N1-C2	9.39	130.74	125.10
58	bO	73	G	C6-N1-C2	9.39	130.73	125.10
58	bO	5	G	C6-N1-C2	9.38	130.73	125.10
55	bK	13	G	C6-N1-C2	9.36	130.72	125.10
55	bK	26	G	C6-N1-C2	9.35	130.71	125.10
55	bK	19	G	C6-N1-C2	9.34	130.70	125.10
58	bO	48	G	C6-N1-C2	9.32	130.69	125.10
55	bK	4	G	C6-N1-C2	9.28	130.67	125.10
47	b4	7	G	C6-N1-C2	9.28	130.66	125.10
58	bO	68	G	C6-N1-C2	9.24	130.64	125.10
58	bO	4	G	C6-N1-C2	9.21	130.62	125.10
62	bS	29	U	N1-C1'-C2'	9.19	125.95	114.00
47	b4	21	U	N3-C4-C5	-9.18	109.09	114.60
47	b4	27	U	N3-C4-C5	-9.16	109.11	114.60
56	bL	46	U	N3-C4-C5	-9.14	109.12	114.60
57	bN	5	U	N3-C4-C5	-9.12	109.13	114.60
57	bN	10	G	C6-N1-C2	9.10	130.56	125.10
55	bK	15	U	N3-C4-C5	-9.08	109.15	114.60
54	bJ	63	C	N1-C1'-C2'	-9.06	102.03	112.00
58	bO	9	G	C6-N1-C2	9.06	130.54	125.10
49	bD	22	U	C2-N3-C4	9.05	132.43	127.00
62	bS	5	U	N1-C2-N3	9.05	120.33	114.90
55	bK	15	U	C2-N3-C4	9.02	132.41	127.00
49	bD	20	U	C2-N3-C4	8.97	132.38	127.00
62	bS	30	U	O4'-C1'-N1	8.96	115.37	108.20
58	bO	79	U	N3-C4-C5	-8.95	109.23	114.60
58	bO	7	U	N3-C4-C5	-8.93	109.25	114.60
57	bN	9	U	N3-C4-C5	-8.88	109.28	114.60
58	bO	8	U	N3-C4-C5	-8.87	109.28	114.60
47	b4	8	U	N3-C4-C5	-8.86	109.28	114.60
58	bO	81	U	N3-C4-C5	-8.85	109.29	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	bK	28	U	N3-C4-C5	-8.84	109.30	114.60
55	bK	65	U	N3-C4-C5	-8.84	109.30	114.60
58	bO	17	U	N3-C4-C5	-8.84	109.30	114.60
58	bO	49	U	N3-C4-C5	-8.84	109.30	114.60
56	bL	25	U	N3-C4-C5	-8.83	109.30	114.60
58	bO	33	U	N3-C4-C5	-8.80	109.32	114.60
58	bO	89	U	N3-C4-C5	-8.80	109.32	114.60
55	bK	5	U	N3-C4-C5	-8.79	109.33	114.60
58	bO	35	U	N3-C4-C5	-8.79	109.33	114.60
58	bO	98	U	N3-C4-C5	-8.79	109.33	114.60
58	bO	85	U	N3-C4-C5	-8.75	109.35	114.60
55	bK	6	U	N3-C4-C5	-8.72	109.37	114.60
49	bD	27	G	C6-N1-C2	8.70	130.32	125.10
63	bT	52	A	C5-C6-N1	8.41	121.91	117.70
54	bJ	8	G	C6-N1-C2	8.33	130.10	125.10
29	BV	225	TYR	CB-CG-CD2	8.30	125.98	121.00
49	bD	21	U	N3-C4-C5	-8.30	109.62	114.60
49	bD	20	U	N3-C4-C5	-8.24	109.66	114.60
58	bO	6	C	C6-N1-C2	-8.17	117.03	120.30
49	bD	22	U	N3-C4-C5	-8.15	109.71	114.60
4	B3	6	TYR	CB-CG-CD2	8.06	125.83	121.00
62	bS	28	U	N1-C1'-C2'	7.98	124.37	114.00
55	bK	14	C	N3-C4-C5	-7.95	118.72	121.90
61	bR	2	G	C6-N1-C2	7.94	129.87	125.10
63	bT	50	A	O4'-C1'-N9	7.93	114.55	108.20
47	b4	25	C	C6-N1-C2	-7.85	117.16	120.30
55	bK	1	A	C8-N9-C4	-7.76	102.70	105.80
55	bK	16	G	C8-N9-C4	-7.75	103.30	106.40
57	bN	10	G	C8-N9-C4	-7.73	103.31	106.40
56	bL	48	G	C8-N9-C4	-7.68	103.33	106.40
56	bL	47	C	C6-N1-C2	-7.67	117.23	120.30
58	bO	9	G	C8-N9-C4	-7.64	103.34	106.40
50	bE	85	U	N3-C2-O2	-7.63	116.86	122.20
57	bN	7	C	C6-N1-C2	-7.56	117.28	120.30
63	bT	49	A	N1-C6-N6	-7.54	114.08	118.60
3	B2	225	ARG	NE-CZ-NH2	7.53	124.06	120.30
54	bJ	65	A	C5-C6-N1	7.51	121.45	117.70
58	bO	5	G	C8-N9-C4	-7.47	103.41	106.40
47	b4	13	C	C6-N1-C2	-7.45	117.32	120.30
58	bO	6	C	C5-C6-N1	7.43	124.72	121.00
55	bK	63	C	C6-N1-C2	-7.43	117.33	120.30
58	bO	82	C	C6-N1-C2	-7.43	117.33	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	bN	6	G	C8-N9-C4	-7.41	103.44	106.40
47	b4	26	G	C8-N9-C4	-7.41	103.44	106.40
12	BB	172	TYR	CB-CG-CD2	7.39	125.43	121.00
57	bN	5	U	C5-C6-N1	7.36	126.38	122.70
47	b4	17	G	C8-N9-C4	-7.32	103.47	106.40
47	b4	18	A	C8-N9-C4	-7.31	102.88	105.80
62	bS	25	U	N3-C2-O2	-7.30	117.09	122.20
62	bS	21	U	N3-C2-O2	-7.29	117.09	122.20
57	bN	8	C	C6-N1-C2	-7.29	117.39	120.30
58	bO	83	C	C6-N1-C2	-7.29	117.39	120.30
21	BK	46	TYR	CB-CG-CD2	7.26	125.36	121.00
55	bK	27	C	C6-N1-C2	-7.25	117.40	120.30
58	bO	92	C	C6-N1-C2	-7.25	117.40	120.30
55	bK	26	G	C8-N9-C4	-7.24	103.50	106.40
37	Bg	80	TYR	CB-CG-CD2	7.22	125.33	121.00
41	Bl	124	TYR	CB-CG-CD2	7.22	125.33	121.00
58	bO	8	U	C5-C6-N1	7.22	126.31	122.70
62	bS	18	U	C1'-O4'-C4'	-7.17	104.16	109.90
55	bK	13	G	C8-N9-C4	-7.17	103.53	106.40
58	bO	68	G	C8-N9-C4	-7.17	103.53	106.40
62	bS	29	U	N3-C2-O2	-7.15	117.19	122.20
54	bJ	63	C	N3-C2-O2	-7.09	116.94	121.90
62	bS	5	U	N3-C2-O2	-7.07	117.25	122.20
47	b4	20	G	C8-N9-C4	-7.07	103.57	106.40
47	b4	25	C	N3-C4-C5	-7.07	119.07	121.90
63	bT	51	A	C5-C6-N1	7.05	121.23	117.70
56	bL	45	G	C8-N9-C4	-7.05	103.58	106.40
63	bT	49	A	C5-C6-N1	7.05	121.23	117.70
47	b4	7	G	C8-N9-C4	-7.04	103.59	106.40
58	bO	87	C	C6-N1-C2	-7.03	117.49	120.30
58	bO	91	C	C6-N1-C2	-7.03	117.49	120.30
55	bK	2	C	N3-C4-C5	-7.02	119.09	121.90
56	bL	24	A	C8-N9-C4	-7.02	102.99	105.80
15	BE	934	LEU	C-N-CD	-7.01	105.18	120.60
58	bO	96	C	C6-N1-C2	-7.01	117.50	120.30
58	bO	88	A	C8-N9-C4	-6.99	103.00	105.80
52	bH	1	U	C5-C6-N1	-6.99	119.21	122.70
56	bL	27	A	C8-N9-C4	-6.97	103.01	105.80
57	bN	11	G	C8-N9-C4	-6.97	103.61	106.40
58	bO	2	G	C8-N9-C4	-6.96	103.62	106.40
47	b4	4	G	C8-N9-C4	-6.95	103.62	106.40
58	bO	80	A	C8-N9-C4	-6.94	103.02	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	b4	23	A	C8-N9-C4	-6.94	103.03	105.80
49	bD	27	G	C8-N9-C4	-6.94	103.62	106.40
47	b4	3	G	C8-N9-C4	-6.93	103.63	106.40
58	bO	34	A	C8-N9-C4	-6.93	103.03	105.80
50	bE	85	U	O4'-C1'-N1	6.93	113.75	108.20
56	bL	47	C	N3-C4-C5	-6.93	119.13	121.90
58	bO	79	U	C5-C6-N1	6.93	126.16	122.70
63	bT	50	A	N1-C6-N6	-6.92	114.45	118.60
58	bO	4	G	C8-N9-C4	-6.91	103.63	106.40
55	bK	61	A	C8-N9-C4	-6.91	103.04	105.80
15	BE	396	PHE	CB-CG-CD2	6.91	125.63	120.80
58	bO	48	G	C8-N9-C4	-6.90	103.64	106.40
47	b4	16	G	C8-N9-C4	-6.89	103.64	106.40
56	bL	44	A	C8-N9-C4	-6.89	103.04	105.80
55	bK	19	G	C8-N9-C4	-6.88	103.65	106.40
62	bS	22	U	N1-C1'-C2'	6.88	122.94	114.00
47	b4	5	A	C8-N9-C4	-6.86	103.05	105.80
58	bO	6	C	N3-C4-C5	-6.85	119.16	121.90
58	bO	16	C	C6-N1-C2	-6.85	117.56	120.30
14	BD	388	PHE	CB-CG-CD2	6.84	125.59	120.80
58	bO	73	G	C8-N9-C4	-6.84	103.67	106.40
57	bN	43	A	C8-N9-C4	-6.84	103.07	105.80
62	bS	22	U	O3'-P-O5'	6.83	116.98	104.00
57	bN	45	A	C8-N9-C4	-6.82	103.07	105.80
58	bO	69	A	C8-N9-C4	-6.82	103.07	105.80
46	b3	3	U	OP1-P-OP2	-6.81	109.38	119.60
57	bN	9	U	C5-C6-N1	6.81	126.10	122.70
47	b4	27	U	C5-C6-N1	6.80	126.10	122.70
46	b3	4	U	OP1-P-OP2	-6.80	109.40	119.60
56	bL	23	A	C8-N9-C4	-6.80	103.08	105.80
47	b4	12	G	C8-N9-C4	-6.80	103.68	106.40
65	bV	1	U	OP1-P-OP2	-6.79	109.41	119.60
14	BD	199	ARG	CD-NE-CZ	6.79	133.11	123.60
65	bV	6	U	OP1-P-OP2	-6.79	109.41	119.60
55	bK	15	U	N3-C4-O4	6.79	124.15	119.40
25	BQ	328	PHE	CB-CG-CD2	6.78	125.54	120.80
30	BW	322	ARG	CD-NE-CZ	6.78	133.09	123.60
63	bT	48	A	N1-C6-N6	-6.76	114.55	118.60
14	BD	391	ARG	CD-NE-CZ	6.76	133.06	123.60
12	BB	282	ARG	CD-NE-CZ	6.75	133.05	123.60
58	bO	84	A	C8-N9-C4	-6.75	103.10	105.80
54	bJ	34	U	OP1-P-OP2	-6.75	109.48	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	BF	259	ARG	CD-NE-CZ	6.74	133.04	123.60
58	bO	101	A	C8-N9-C4	-6.74	103.10	105.80
12	BB	1153	ARG	CD-NE-CZ	6.74	133.04	123.60
30	BW	279	ARG	CD-NE-CZ	6.74	133.04	123.60
37	Bg	170	ARG	CD-NE-CZ	6.73	133.03	123.60
58	bO	102	A	C8-N9-C4	-6.73	103.11	105.80
55	bK	27	C	C5-C6-N1	6.73	124.36	121.00
15	BE	394	ARG	CD-NE-CZ	6.72	133.01	123.60
55	bK	14	C	C5-C6-N1	6.72	124.36	121.00
55	bK	63	C	N3-C4-C5	-6.72	119.21	121.90
58	bO	100	A	C8-N9-C4	-6.72	103.11	105.80
58	bO	50	A	C8-N9-C4	-6.72	103.11	105.80
54	bJ	12	A	OP1-P-OP2	-6.72	109.53	119.60
58	bO	1	A	C8-N9-C4	-6.72	103.11	105.80
14	BD	207	ARG	CD-NE-CZ	6.71	133.00	123.60
58	bO	90	A	C8-N9-C4	-6.71	103.11	105.80
12	BB	160	ARG	CD-NE-CZ	6.71	132.99	123.60
18	BH	64	ARG	CD-NE-CZ	6.71	132.99	123.60
42	HJ	751	ARG	CD-NE-CZ	6.71	132.99	123.60
42	HJ	759	ARG	CD-NE-CZ	6.71	132.99	123.60
16	BF	274	ARG	CD-NE-CZ	6.70	132.98	123.60
42	HJ	685	ARG	CD-NE-CZ	6.70	132.98	123.60
53	bI	2	U	C4-C5-C6	6.70	123.72	119.70
55	bK	64	A	C8-N9-C4	-6.70	103.12	105.80
27	BT	62	ARG	CD-NE-CZ	6.70	132.98	123.60
58	bO	10	A	C8-N9-C4	-6.70	103.12	105.80
57	bN	8	C	N3-C4-C5	-6.70	119.22	121.90
14	BD	257	ARG	CD-NE-CZ	6.70	132.97	123.60
12	BB	1115	TYR	CB-CG-CD2	6.69	125.01	121.00
58	bO	82	C	N3-C4-C5	-6.68	119.23	121.90
58	bO	93	A	C8-N9-C4	-6.68	103.13	105.80
37	Bg	162	ARG	CD-NE-CZ	6.68	132.95	123.60
12	BB	670	ARG	CD-NE-CZ	6.68	132.95	123.60
63	bT	52	A	C4-C5-C6	-6.68	113.66	117.00
1	B0	36	ARG	CD-NE-CZ	6.67	132.94	123.60
16	BF	33	ARG	CD-NE-CZ	6.67	132.94	123.60
61	bR	2	G	C8-N9-C4	-6.67	103.73	106.40
58	bO	83	C	N3-C4-C5	-6.67	119.23	121.90
14	BD	368	ARG	CD-NE-CZ	6.67	132.94	123.60
14	BD	387	ARG	CD-NE-CZ	6.67	132.94	123.60
42	HJ	733	PHE	CB-CG-CD2	6.67	125.47	120.80
47	b4	13	C	N3-C4-C5	-6.67	119.23	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B0	150	ARG	CD-NE-CZ	6.67	132.93	123.60
13	BC	203	ARG	CD-NE-CZ	6.66	132.93	123.60
42	HJ	639	ARG	CD-NE-CZ	6.66	132.92	123.60
62	bS	18	U	C5'-C4'-O4'	6.65	117.08	109.10
10	B9	59	ARG	CD-NE-CZ	6.65	132.91	123.60
41	Bl	14	ARG	CD-NE-CZ	6.65	132.91	123.60
40	Bk	34	ARG	CD-NE-CZ	6.64	132.90	123.60
58	bO	31	A	C8-N9-C4	-6.64	103.14	105.80
58	bO	74	A	C8-N9-C4	-6.64	103.14	105.80
13	BC	42	ARG	CD-NE-CZ	6.64	132.90	123.60
42	HJ	730	ARG	CD-NE-CZ	6.64	132.90	123.60
27	BT	44	ARG	CD-NE-CZ	6.64	132.90	123.60
58	bO	92	C	N3-C4-C5	-6.64	119.24	121.90
15	BE	492	ARG	CD-NE-CZ	6.63	132.89	123.60
58	bO	4	G	C5-N7-C8	-6.63	100.98	104.30
12	BB	68	ARG	CD-NE-CZ	6.63	132.88	123.60
1	B0	271	ARG	CD-NE-CZ	6.63	132.88	123.60
30	BW	286	ARG	CD-NE-CZ	6.63	132.88	123.60
30	BW	320	ARG	CD-NE-CZ	6.63	132.88	123.60
12	BB	426	ARG	CD-NE-CZ	6.63	132.88	123.60
25	BQ	469	ARG	CD-NE-CZ	6.62	132.88	123.60
58	bO	16	C	N3-C4-C5	-6.62	119.25	121.90
55	bK	15	U	C5-C6-N1	6.62	126.01	122.70
58	bO	91	C	N3-C4-C5	-6.62	119.25	121.90
30	BW	315	ARG	CD-NE-CZ	6.62	132.86	123.60
13	BC	43	ARG	CD-NE-CZ	6.62	132.86	123.60
55	bK	20	A	C8-N9-C4	-6.62	103.15	105.80
1	B0	268	ARG	CD-NE-CZ	6.61	132.86	123.60
13	BC	208	ARG	CD-NE-CZ	6.61	132.85	123.60
58	bO	87	C	N3-C4-C5	-6.60	119.26	121.90
25	BQ	410	ARG	CD-NE-CZ	6.60	132.84	123.60
49	bD	21	U	C5-C6-N1	6.60	126.00	122.70
27	BT	79	ARG	CD-NE-CZ	6.60	132.84	123.60
58	bO	85	U	C5-C6-N1	6.60	126.00	122.70
57	bN	48	G	N3-C2-N2	-6.59	115.29	119.90
1	B0	249	ARG	CD-NE-CZ	6.58	132.81	123.60
58	bO	3	A	C8-N9-C4	-6.58	103.17	105.80
56	bL	26	A	C8-N9-C4	-6.57	103.17	105.80
55	bK	4	G	C8-N9-C4	-6.57	103.77	106.40
12	BB	61	ARG	CD-NE-CZ	6.56	132.78	123.60
58	bO	32	A	C8-N9-C4	-6.55	103.18	105.80
58	bO	58	A	C8-N9-C4	-6.54	103.18	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	BD	93	ARG	CD-NE-CZ	6.53	132.75	123.60
57	bN	7	C	N3-C4-C5	-6.53	119.29	121.90
40	Bk	51	ARG	CD-NE-CZ	6.53	132.74	123.60
55	bK	62	A	C8-N9-C4	-6.53	103.19	105.80
58	bO	7	U	C5-C6-N1	6.53	125.96	122.70
57	bN	46	A	C8-N9-C4	-6.52	103.19	105.80
58	bO	99	A	C8-N9-C4	-6.52	103.19	105.80
63	bT	50	A	C5-C6-N1	6.52	120.96	117.70
52	bH	2	U	N3-C2-O2	-6.52	117.64	122.20
55	bK	66	A	C8-N9-C4	-6.52	103.19	105.80
58	bO	96	C	N3-C4-C5	-6.51	119.29	121.90
62	bS	31	U	N3-C2-O2	-6.51	117.64	122.20
37	Bg	176	ARG	CD-NE-CZ	6.49	132.68	123.60
49	bD	22	U	C5-C6-N1	6.48	125.94	122.70
58	bO	89	U	C5-C6-N1	6.48	125.94	122.70
16	BF	248	TYR	CB-CG-CD2	6.48	124.89	121.00
1	B0	171	ARG	CD-NE-CZ	6.47	132.66	123.60
61	bR	3	A	C8-N9-C4	-6.47	103.21	105.80
55	bK	65	U	C5-C6-N1	6.46	125.93	122.70
47	b4	25	C	C5-C6-N1	6.44	124.22	121.00
63	bT	51	A	C4-C5-C6	-6.44	113.78	117.00
55	bK	2	C	C3'-C2'-C1'	6.43	106.64	101.50
56	bL	46	U	C5-C6-N1	6.43	125.91	122.70
57	bN	44	A	C8-N9-C4	-6.42	103.23	105.80
30	BW	321	ARG	CD-NE-CZ	6.42	132.59	123.60
55	bK	27	C	N3-C4-C5	-6.42	119.33	121.90
63	bT	48	A	C5-C6-N1	6.41	120.91	117.70
58	bO	81	U	C5-C6-N1	6.41	125.91	122.70
47	b4	21	U	C5-C6-N1	6.41	125.90	122.70
1	B0	242	ARG	CD-NE-CZ	6.41	132.57	123.60
47	b4	8	U	C5-C6-N1	6.40	125.90	122.70
58	bO	17	U	C5-C6-N1	6.40	125.90	122.70
15	BE	765	ARG	CD-NE-CZ	6.40	132.56	123.60
55	bK	23	A	C5-C6-N1	6.38	120.89	117.70
58	bO	49	U	C5-C6-N1	6.37	125.88	122.70
39	Bi	128	ARG	CD-NE-CZ	6.36	132.50	123.60
55	bK	5	U	C5-C6-N1	6.34	125.87	122.70
58	bO	4	G	N1-C6-O6	6.34	123.70	119.90
25	BQ	373	ARG	CD-NE-CZ	6.33	132.46	123.60
58	bO	98	U	C5-C6-N1	6.32	125.86	122.70
55	bK	28	U	C5-C6-N1	6.32	125.86	122.70
40	Bk	275	ARG	NE-CZ-NH2	6.32	123.46	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	Bg	83	MET	CA-CB-CG	6.30	124.01	113.30
58	bO	12	A	N1-C6-N6	-6.29	114.82	118.60
15	BE	941	ARG	NE-CZ-NH2	6.29	123.45	120.30
49	bD	26	A	C8-N9-C4	-6.28	103.29	105.80
56	bL	47	C	C5-C6-N1	6.28	124.14	121.00
1	B0	187	TYR	CB-CG-CD2	6.28	124.77	121.00
64	bU	18	U	N3-C2-O2	-6.28	117.81	122.20
55	bK	6	U	C5-C6-N1	6.28	125.84	122.70
47	b4	18	A	C5-N7-C8	-6.27	100.77	103.90
15	BE	932	ARG	NE-CZ-NH2	6.25	123.43	120.30
64	bU	18	U	N1-C2-N3	6.24	118.64	114.90
58	bO	35	U	C5-C6-N1	6.22	125.81	122.70
62	bS	29	U	N1-C2-N3	6.21	118.63	114.90
58	bO	5	G	C5-N7-C8	-6.18	101.21	104.30
58	bO	33	U	C5-C6-N1	6.17	125.79	122.70
49	bD	20	U	C5-C6-N1	6.16	125.78	122.70
15	BE	1050	ARG	NE-CZ-NH2	6.15	123.37	120.30
55	bK	16	G	C5-N7-C8	-6.15	101.23	104.30
57	bN	50	A	N1-C6-N6	-6.13	114.92	118.60
15	BE	845	ARG	CD-NE-CZ	6.12	132.18	123.60
58	bO	82	C	C5-C6-N1	6.12	124.06	121.00
55	bK	3	A	C8-N9-C4	-6.11	103.36	105.80
15	BE	411	PHE	CB-CG-CD2	6.11	125.08	120.80
57	bN	8	C	C5-C6-N1	6.10	124.05	121.00
55	bK	63	C	C5-C6-N1	6.07	124.03	121.00
62	bS	18	U	O5'-C5'-C4'	6.06	123.22	111.70
1	B0	154	MET	CA-CB-CG	6.06	123.60	113.30
11	BA	129	ARG	CD-NE-CZ	6.06	132.08	123.60
7	B6	63	ARG	CD-NE-CZ	6.05	132.07	123.60
7	B6	12	ARG	CD-NE-CZ	6.05	132.07	123.60
7	B6	91	ARG	CD-NE-CZ	6.04	132.05	123.60
58	bO	83	C	C5-C6-N1	6.04	124.02	121.00
55	bK	2	C	C6-N1-C2	-6.03	117.89	120.30
27	BT	14	ARG	CD-NE-CZ	6.02	132.03	123.60
21	BK	53	MET	CA-CB-CG	6.02	123.53	113.30
47	b4	13	C	C5-C6-N1	6.02	124.01	121.00
7	B6	45	ARG	CD-NE-CZ	6.02	132.02	123.60
47	b4	23	A	C2-N3-C4	-6.02	107.59	110.60
55	bK	3	A	C5-N7-C8	-6.01	100.89	103.90
56	bL	48	G	C5-N7-C8	-6.01	101.30	104.30
30	BW	281	PHE	CB-CG-CD2	6.01	125.00	120.80
39	Bi	124	TYR	CB-CG-CD2	6.00	124.60	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	bJ	8	G	C8-N9-C4	-6.00	104.00	106.40
21	BK	58	PHE	CB-CG-CD2	5.99	125.00	120.80
47	b4	18	A	C2-N3-C4	-5.99	107.60	110.60
38	Bh	131	TYR	CB-CG-CD2	5.99	124.59	121.00
57	bN	7	C	C5-C6-N1	5.99	124.00	121.00
40	Bk	16	ARG	CD-NE-CZ	5.99	131.98	123.60
42	HJ	734	TYR	CB-CG-CD2	5.98	124.59	121.00
55	bK	3	A	C6-N1-C2	-5.98	115.01	118.60
56	bL	25	U	C5-C6-N1	5.98	125.69	122.70
22	BL	85	ARG	CD-NE-CZ	5.97	131.96	123.60
62	bS	18	U	P-O3'-C3'	5.97	126.86	119.70
42	HJ	724	MET	CA-CB-CG	5.96	123.43	113.30
56	bL	44	A	C5-N7-C8	-5.96	100.92	103.90
62	bS	28	U	N3-C2-O2	-5.96	118.03	122.20
30	BW	101	ARG	CD-NE-CZ	5.95	131.93	123.60
15	BE	523	ARG	CD-NE-CZ	5.95	131.93	123.60
22	BL	45	ARG	CD-NE-CZ	5.95	131.92	123.60
22	BL	78	ARG	CD-NE-CZ	5.94	131.92	123.60
56	bL	44	A	C2-N3-C4	-5.94	107.63	110.60
58	bO	92	C	C5-C6-N1	5.94	123.97	121.00
15	BE	488	MET	CA-CB-CG	5.94	123.40	113.30
47	b4	5	A	C2-N3-C4	-5.94	107.63	110.60
15	BE	921	ARG	NE-CZ-NH2	5.94	123.27	120.30
4	B3	221	ARG	CD-NE-CZ	5.93	131.90	123.60
39	Bi	86	ARG	CD-NE-CZ	5.93	131.90	123.60
57	bN	6	G	C5-N7-C8	-5.93	101.33	104.30
3	B2	108	ARG	CD-NE-CZ	5.93	131.90	123.60
3	B2	4	ARG	CD-NE-CZ	5.92	131.89	123.60
55	bK	13	G	C5-N7-C8	-5.92	101.34	104.30
47	b4	20	G	C5-N7-C8	-5.92	101.34	104.30
25	BQ	68	ARG	CD-NE-CZ	5.91	131.88	123.60
58	bO	74	A	C2-N3-C4	-5.91	107.64	110.60
56	bL	45	G	C5-N7-C8	-5.91	101.35	104.30
58	bO	88	A	C2-N3-C4	-5.91	107.65	110.60
16	BF	37	PHE	CB-CG-CD2	5.91	124.93	120.80
30	BW	196	TYR	CB-CG-CD2	5.91	124.54	121.00
55	bK	1	A	C5-N7-C8	-5.91	100.95	103.90
55	bK	26	G	C5-N7-C8	-5.90	101.35	104.30
54	bJ	65	A	C4-C5-C6	-5.90	114.05	117.00
62	bS	23	U	C5-C6-N1	-5.89	119.75	122.70
58	bO	87	C	C5-C6-N1	5.89	123.94	121.00
58	bO	96	C	C5-C6-N1	5.89	123.94	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	bO	99	A	C2-N3-C4	-5.89	107.66	110.60
55	bK	14	C	C4-C5-C6	5.89	120.34	117.40
16	BF	19	MET	CA-CB-CG	5.89	123.31	113.30
3	B2	46	ARG	CD-NE-CZ	5.88	131.83	123.60
57	bN	46	A	C2-N3-C4	-5.88	107.66	110.60
50	bE	85	U	N1-C2-O2	5.88	126.91	122.80
47	b4	23	A	C5-N7-C8	-5.88	100.96	103.90
58	bO	50	A	C2-N3-C4	-5.87	107.66	110.60
47	b4	26	G	C5-N7-C8	-5.87	101.37	104.30
12	BB	181	PHE	CB-CG-CD2	5.86	124.90	120.80
29	BV	223	MET	CA-CB-CG	5.86	123.27	113.30
58	bO	84	A	C2-N3-C4	-5.86	107.67	110.60
3	B2	148	ARG	CD-NE-CZ	5.86	131.80	123.60
58	bO	91	C	C5-C6-N1	5.86	123.93	121.00
55	bK	61	A	C5-N7-C8	-5.85	100.97	103.90
57	bN	44	A	C2-N3-C4	-5.85	107.67	110.60
55	bK	16	G	C5-C6-N1	-5.84	108.58	111.50
55	bK	20	A	C2-N3-C4	-5.84	107.68	110.60
57	bN	10	G	C5-N7-C8	-5.84	101.38	104.30
47	b4	5	A	C5-N7-C8	-5.83	100.98	103.90
55	bK	64	A	C2-N3-C4	-5.83	107.68	110.60
58	bO	3	A	C2-N3-C4	-5.83	107.69	110.60
57	bN	45	A	C5-N7-C8	-5.83	100.99	103.90
1	B0	45	TYR	CB-CG-CD2	5.82	124.49	121.00
55	bK	64	A	C5-N7-C8	-5.81	101.00	103.90
55	bK	62	A	C2-N3-C4	-5.81	107.70	110.60
58	bO	9	G	C5-N7-C8	-5.81	101.40	104.30
56	bL	24	A	C2-N3-C4	-5.81	107.70	110.60
58	bO	100	A	C2-N3-C4	-5.80	107.70	110.60
62	bS	31	U	N1-C2-N3	5.80	118.38	114.90
55	bK	61	A	C2-N3-C4	-5.80	107.70	110.60
58	bO	10	A	C5-N7-C8	-5.80	101.00	103.90
12	BB	259	TYR	CB-CG-CD2	5.79	124.47	121.00
57	bN	43	A	C5-N7-C8	-5.79	101.00	103.90
56	bL	23	A	C2-N3-C4	-5.79	107.71	110.60
56	bL	27	A	C5-N7-C8	-5.78	101.01	103.90
58	bO	93	A	C2-N3-C4	-5.78	107.71	110.60
58	bO	90	A	C2-N3-C4	-5.78	107.71	110.60
12	BB	952	ARG	CD-NE-CZ	5.78	131.69	123.60
56	bL	26	A	C2-N3-C4	-5.78	107.71	110.60
12	BB	983	ARG	CD-NE-CZ	5.78	131.69	123.60
58	bO	80	A	C5-N7-C8	-5.78	101.01	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	bS	22	U	C4'-C3'-C2'	-5.78	96.83	102.60
12	BB	1007	ARG	CD-NE-CZ	5.77	131.68	123.60
58	bO	102	A	C5-N7-C8	-5.77	101.02	103.90
3	B2	264	TYR	CB-CG-CD2	5.76	124.46	121.00
55	bK	20	A	C5-N7-C8	-5.76	101.02	103.90
58	bO	74	A	C5-N7-C8	-5.76	101.02	103.90
47	b4	4	G	C5-N7-C8	-5.76	101.42	104.30
57	bN	45	A	C2-N3-C4	-5.76	107.72	110.60
58	bO	32	A	C2-N3-C4	-5.75	107.72	110.60
58	bO	1	A	C2-N3-C4	-5.75	107.72	110.60
58	bO	34	A	C5-N7-C8	-5.75	101.03	103.90
58	bO	90	A	C5-N7-C8	-5.75	101.03	103.90
62	bS	21	U	O4'-C1'-C2'	-5.75	100.05	105.80
12	BB	1112	ARG	CD-NE-CZ	5.75	131.65	123.60
47	b4	17	G	C5-N7-C8	-5.75	101.43	104.30
57	bN	43	A	C2-N3-C4	-5.75	107.73	110.60
3	B2	284	MET	CA-CB-CG	5.74	123.06	113.30
55	bK	23	A	N1-C6-N6	-5.74	115.15	118.60
58	bO	58	A	C2-N3-C4	-5.74	107.73	110.60
58	bO	58	A	C5-N7-C8	-5.74	101.03	103.90
58	bO	88	A	C5-N7-C8	-5.74	101.03	103.90
58	bO	101	A	C2-N3-C4	-5.74	107.73	110.60
57	bN	46	A	C5-N7-C8	-5.74	101.03	103.90
14	BD	151	ARG	CD-NE-CZ	5.74	131.64	123.60
56	bL	23	A	C5-N7-C8	-5.74	101.03	103.90
14	BD	3	ARG	CD-NE-CZ	5.74	131.63	123.60
56	bL	24	A	C5-N7-C8	-5.74	101.03	103.90
58	bO	31	A	C2-N3-C4	-5.74	107.73	110.60
58	bO	32	A	C5-N7-C8	-5.73	101.03	103.90
30	BW	313	MET	CA-CB-CG	5.73	123.04	113.30
58	bO	31	A	C5-N7-C8	-5.73	101.04	103.90
55	bK	62	A	C5-N7-C8	-5.72	101.04	103.90
56	bL	45	G	C5-C6-N1	-5.72	108.64	111.50
58	bO	84	A	C5-N7-C8	-5.72	101.04	103.90
56	bL	48	G	C5-C6-N1	-5.72	108.64	111.50
55	bK	2	C	C5-C6-N1	5.72	123.86	121.00
57	bN	44	A	C5-N7-C8	-5.71	101.04	103.90
52	bH	1	U	C4-C5-C6	5.71	123.13	119.70
58	bO	1	A	C5-N7-C8	-5.71	101.05	103.90
15	BE	819	MET	CA-CB-CG	5.71	123.00	113.30
58	bO	80	A	C2-N3-C4	-5.71	107.75	110.60
47	b4	20	G	C5-C6-N1	-5.71	108.65	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	bO	93	A	C5-N7-C8	-5.70	101.05	103.90
58	bO	99	A	C5-N7-C8	-5.70	101.05	103.90
12	BB	948	ARG	CD-NE-CZ	5.70	131.58	123.60
47	b4	26	G	C5-C6-N1	-5.70	108.65	111.50
37	Bg	63	PHE	CB-CG-CD2	5.70	124.79	120.80
58	bO	101	A	C5-N7-C8	-5.69	101.05	103.90
12	BB	1108	ARG	CD-NE-CZ	5.69	131.57	123.60
58	bO	10	A	C2-N3-C4	-5.69	107.76	110.60
58	bO	16	C	C5-C6-N1	5.68	123.84	121.00
14	BD	211	TYR	CB-CG-CD2	5.68	124.41	121.00
55	bK	66	A	C3'-C2'-C1'	5.68	106.04	101.50
55	bK	66	A	C5-N7-C8	-5.68	101.06	103.90
58	bO	50	A	C5-N7-C8	-5.67	101.06	103.90
58	bO	102	A	C2-N3-C4	-5.67	107.77	110.60
56	bL	26	A	C5-N7-C8	-5.66	101.07	103.90
62	bS	30	U	N1-C2-N3	5.66	118.30	114.90
25	BQ	366	ARG	CD-NE-CZ	5.66	131.52	123.60
47	b4	3	G	C5-N7-C8	-5.65	101.47	104.30
57	bN	5	U	C6-N1-C2	-5.65	117.61	121.00
58	bO	73	G	C5-N7-C8	-5.65	101.47	104.30
15	BE	923	ARG	NE-CZ-NH2	5.64	123.12	120.30
47	b4	12	G	C5-N7-C8	-5.64	101.48	104.30
58	bO	48	G	C5-N7-C8	-5.64	101.48	104.30
15	BE	1044	ARG	NE-CZ-NH2	5.64	123.12	120.30
55	bK	2	C	C4-C5-C6	5.64	120.22	117.40
58	bO	3	A	C5-N7-C8	-5.64	101.08	103.90
12	BB	1022	ARG	CD-NE-CZ	5.63	131.48	123.60
56	bL	47	C	C4-C5-C6	5.63	120.22	117.40
58	bO	100	A	C5-N7-C8	-5.63	101.09	103.90
38	Bh	8	PHE	CB-CG-CD2	5.63	124.74	120.80
58	bO	69	A	C2-N3-C4	-5.62	107.79	110.60
42	HJ	604	ARG	CD-NE-CZ	5.62	131.47	123.60
1	B0	163	TYR	CB-CG-CD2	5.62	124.37	121.00
37	Bg	74	PHE	CB-CG-CD2	5.62	124.73	120.80
47	b4	16	G	C5-N7-C8	-5.61	101.49	104.30
56	bL	27	A	C2-N3-C4	-5.61	107.79	110.60
55	bK	19	G	C5-N7-C8	-5.61	101.50	104.30
37	Bg	46	PHE	CB-CG-CD2	5.61	124.72	120.80
58	bO	2	G	C5-N7-C8	-5.60	101.50	104.30
47	b4	7	G	C5-N7-C8	-5.60	101.50	104.30
14	BD	216	ARG	CD-NE-CZ	5.60	131.44	123.60
57	bN	50	A	C5-C6-N1	5.59	120.50	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	bO	34	A	C2-N3-C4	-5.59	107.81	110.60
55	bK	26	G	C5-C6-N1	-5.58	108.71	111.50
57	bN	11	G	C5-C6-N1	-5.58	108.71	111.50
57	bN	6	G	C5-C6-N1	-5.58	108.71	111.50
58	bO	5	G	C5-C6-N1	-5.56	108.72	111.50
55	bK	66	A	C2-N3-C4	-5.56	107.82	110.60
30	BW	240	PHE	CB-CG-CD2	5.55	124.69	120.80
3	B2	50	PHE	CB-CG-CD2	5.55	124.69	120.80
61	bR	3	A	C5-N7-C8	-5.54	101.13	103.90
47	b4	25	C	C4-C5-C6	5.53	120.17	117.40
58	bO	68	G	C5-N7-C8	-5.53	101.53	104.30
15	BE	975	ARG	NE-CZ-NH2	5.53	123.06	120.30
47	b4	17	G	C5-C6-N1	-5.53	108.74	111.50
55	bK	1	A	C6-N1-C2	-5.52	115.29	118.60
61	bR	3	A	C2-N3-C4	-5.52	107.84	110.60
47	b4	3	G	C5-C6-N1	-5.52	108.74	111.50
57	bN	11	G	C5-N7-C8	-5.51	101.54	104.30
47	b4	13	C	C4-C5-C6	5.51	120.16	117.40
58	bO	9	G	C5-C6-N1	-5.50	108.75	111.50
47	b4	16	G	C5-C6-N1	-5.50	108.75	111.50
47	b4	4	G	C5-C6-N1	-5.49	108.75	111.50
53	bI	2	U	C5-C6-N1	-5.49	119.95	122.70
55	bK	13	G	C5-C6-N1	-5.49	108.76	111.50
58	bO	2	G	C5-C6-N1	-5.47	108.76	111.50
62	bS	20	U	O4'-C1'-N1	5.47	112.58	108.20
62	bS	27	U	N3-C2-O2	-5.47	118.37	122.20
46	b3	3	U	OP1-P-O3'	5.47	117.24	105.20
58	bO	73	G	C5-C6-N1	-5.46	108.77	111.50
55	bK	4	G	C5-N7-C8	-5.46	101.57	104.30
58	bO	69	A	C5-N7-C8	-5.46	101.17	103.90
47	b4	12	G	C5-C6-N1	-5.45	108.77	111.50
13	BC	44	TYR	CB-CG-CD2	5.45	124.27	121.00
57	bN	8	C	C4-C5-C6	5.45	120.12	117.40
47	b4	7	G	C5-C6-N1	-5.44	108.78	111.50
58	bO	16	C	C4-C5-C6	5.44	120.12	117.40
58	bO	48	G	C5-C6-N1	-5.44	108.78	111.50
55	bK	19	G	C5-C6-N1	-5.43	108.78	111.50
58	bO	8	U	C6-N1-C2	-5.43	117.74	121.00
65	bV	5	U	OP1-P-O3'	5.42	117.13	105.20
42	HJ	717	TYR	CB-CG-CD2	5.42	124.25	121.00
55	bK	63	C	C4-C5-C6	5.42	120.11	117.40
49	bD	26	A	C2-N3-C4	-5.42	107.89	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	bK	10	G	C5-C6-N1	5.42	114.21	111.50
14	BD	210	PHE	CB-CG-CD2	5.42	124.59	120.80
14	BD	257	ARG	CG-CD-NE	5.41	123.16	111.80
1	B0	152	TYR	CB-CG-CD2	5.40	124.24	121.00
14	BD	207	ARG	CG-CD-NE	5.39	123.12	111.80
46	b3	2	U	OP1-P-O3'	5.39	117.05	105.20
42	HJ	759	ARG	CG-CD-NE	5.38	123.10	111.80
51	bG	2	U	C2-N3-C4	-5.38	123.77	127.00
3	B2	123	TYR	CB-CG-CD2	5.38	124.23	121.00
58	bO	4	G	N1-C2-N3	-5.38	120.67	123.90
1	B0	268	ARG	CG-CD-NE	5.37	123.08	111.80
62	bS	28	U	N1-C2-N3	5.37	118.12	114.90
57	bN	7	C	C4-C5-C6	5.37	120.09	117.40
54	bJ	65	A	C2-N3-C4	5.36	113.28	110.60
55	bK	4	G	C5-C6-N1	-5.36	108.82	111.50
49	bD	26	A	C5-N7-C8	-5.36	101.22	103.90
58	bO	92	C	C4-C5-C6	5.36	120.08	117.40
61	bR	2	G	C5-N7-C8	-5.36	101.62	104.30
58	bO	68	G	C5-C6-N1	-5.36	108.82	111.50
16	BF	259	ARG	CG-CD-NE	5.36	123.05	111.80
58	bO	83	C	C4-C5-C6	5.35	120.08	117.40
14	BD	368	ARG	CG-CD-NE	5.35	123.03	111.80
30	BW	322	ARG	CG-CD-NE	5.34	123.01	111.80
58	bO	91	C	C4-C5-C6	5.34	120.07	117.40
18	BH	64	ARG	CG-CD-NE	5.33	123.00	111.80
14	BD	199	ARG	CG-CD-NE	5.33	123.00	111.80
37	Bg	179	PHE	CB-CG-CD2	5.33	124.53	120.80
58	bO	82	C	C4-C5-C6	5.33	120.06	117.40
16	BF	274	ARG	CG-CD-NE	5.32	122.98	111.80
10	B9	59	ARG	CG-CD-NE	5.32	122.97	111.80
58	bO	87	C	C4-C5-C6	5.32	120.06	117.40
14	BD	470	ARG	CD-NE-CZ	5.32	131.04	123.60
16	BF	33	ARG	CG-CD-NE	5.31	122.95	111.80
42	HJ	681	PHE	CB-CG-CD2	5.31	124.52	120.80
54	bJ	61	U	N3-C2-O2	-5.31	118.48	122.20
58	bO	6	C	C4-C5-C6	5.29	120.05	117.40
30	BW	286	ARG	CG-CD-NE	5.29	122.91	111.80
54	bJ	64	U	N3-C2-O2	-5.29	118.50	122.20
3	B2	256	MET	CA-CB-CG	5.29	122.29	113.30
7	B6	106	TYR	CB-CG-CD2	5.29	124.17	121.00
57	bN	10	G	C5-C6-N1	-5.28	108.86	111.50
14	BD	7	ARG	NE-CZ-NH2	5.28	122.94	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	b4	1	A	C5-C6-N1	5.27	120.34	117.70
13	BC	208	ARG	CG-CD-NE	5.27	122.86	111.80
58	bO	96	C	C4-C5-C6	5.27	120.03	117.40
42	HJ	751	ARG	CG-CD-NE	5.27	122.86	111.80
49	bD	27	G	C5-N7-C8	-5.26	101.67	104.30
3	B2	225	ARG	NH1-CZ-NH2	-5.25	113.62	119.40
30	BW	231	PHE	CB-CG-CD2	5.25	124.47	120.80
12	BB	61	ARG	CG-CD-NE	5.25	122.82	111.80
3	B2	149	MET	CA-CB-CG	5.24	122.21	113.30
30	BW	315	ARG	CG-CD-NE	5.23	122.79	111.80
15	BE	868	ARG	NE-CZ-NH2	5.23	122.92	120.30
58	bO	79	U	C6-N1-C2	-5.22	117.87	121.00
58	bO	77	A	N1-C6-N6	-5.22	115.47	118.60
12	BB	68	ARG	CG-CD-NE	5.20	122.71	111.80
12	BB	426	ARG	CG-CD-NE	5.18	122.69	111.80
49	bD	27	G	C5-C6-N1	-5.18	108.91	111.50
54	bJ	64	U	C5-C6-N1	-5.18	120.11	122.70
12	BB	670	ARG	CG-CD-NE	5.17	122.67	111.80
7	B6	104	MET	CA-CB-CG	5.17	122.09	113.30
62	bS	25	U	N1-C2-N3	5.16	118.00	114.90
37	Bg	176	ARG	CG-CD-NE	5.16	122.63	111.80
54	bJ	58	A	C5-C6-N1	5.16	120.28	117.70
15	BE	602	PHE	CB-CG-CD2	5.15	124.41	120.80
63	bT	49	A	C4-C5-C6	-5.15	114.42	117.00
7	B6	66	TYR	CB-CG-CD2	5.14	124.09	121.00
37	Bg	167	PHE	CB-CG-CD2	5.14	124.40	120.80
30	BW	271	PHE	CB-CG-CD2	5.14	124.40	120.80
55	bK	9	C	N3-C2-O2	-5.13	118.31	121.90
47	b4	23	A	C6-N1-C2	-5.13	115.52	118.60
62	bS	22	U	N3-C2-O2	-5.13	118.61	122.20
1	B0	273	ARG	CD-NE-CZ	5.12	130.77	123.60
56	bL	44	A	C6-N1-C2	-5.12	115.53	118.60
57	bN	9	U	C6-N1-C2	-5.12	117.93	121.00
3	B2	288	MET	CA-CB-CG	5.12	122.00	113.30
15	BE	948	ARG	NE-CZ-NH2	5.12	122.86	120.30
47	b4	18	A	C6-N1-C2	-5.11	115.53	118.60
57	bN	39	A	P-O3'-C3'	5.11	125.83	119.70
54	bJ	61	U	C5-C6-N1	-5.11	120.15	122.70
14	BD	165	PHE	CB-CG-CD2	5.10	124.37	120.80
47	b4	27	U	C6-N1-C2	-5.10	117.94	121.00
27	BT	44	ARG	CG-CD-NE	5.10	122.50	111.80
1	B0	305	ARG	CD-NE-CZ	5.09	130.73	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	Bh	129	ARG	CD-NE-CZ	5.09	130.73	123.60
30	BW	303	PHE	CB-CG-CD2	5.09	124.36	120.80
62	bS	16	U	N1-C2-N3	5.09	117.95	114.90
55	bK	15	U	C6-N1-C2	-5.09	117.95	121.00
4	B3	222	MET	CA-CB-CG	5.09	121.95	113.30
11	BA	449	ARG	CD-NE-CZ	5.09	130.72	123.60
58	bO	77	A	O4'-C1'-N9	5.09	112.27	108.20
13	BC	43	ARG	CG-CD-NE	5.08	122.47	111.80
15	BE	945	ARG	NE-CZ-NH2	5.08	122.84	120.30
62	bS	21	U	O4'-C1'-N1	5.08	112.27	108.20
42	HJ	651	PHE	CB-CG-CD2	5.07	124.35	120.80
15	BE	562	PHE	CB-CG-CD2	5.07	124.35	120.80
30	BW	324	ARG	CD-NE-CZ	5.06	130.69	123.60
55	bK	64	A	C6-N1-C2	-5.06	115.56	118.60
11	BA	446	ARG	CD-NE-CZ	5.06	130.68	123.60
55	bK	3	A	C2-N3-C4	-5.06	108.07	110.60
62	bS	29	U	C5-C6-N1	-5.05	120.17	122.70
55	bK	10	G	N3-C4-C5	-5.05	126.07	128.60
49	bD	22	U	N1-C2-N3	-5.05	111.87	114.90
3	B2	134	ARG	CD-NE-CZ	5.05	130.67	123.60
58	bO	7	U	C6-N1-C2	-5.05	117.97	121.00
62	bS	30	U	N3-C2-O2	-5.05	118.67	122.20
54	bJ	8	G	C5-N7-C8	-5.04	101.78	104.30
12	BB	413	ARG	NE-CZ-NH2	5.04	122.82	120.30
11	BA	448	ARG	CD-NE-CZ	5.04	130.65	123.60
54	bJ	61	U	N1-C2-N3	5.04	117.92	114.90
55	bK	10	G	N3-C2-N2	-5.03	116.38	119.90
56	bL	46	U	N1-C2-N3	-5.03	111.88	114.90
5	B4	7	ARG	NE-CZ-NH2	5.03	122.81	120.30
39	Bi	124	TYR	CD1-CG-CD2	-5.03	112.37	117.90
12	BB	1124	ARG	CB-CA-C	5.02	120.44	110.40
15	BE	1045	ARG	NE-CZ-NH2	5.01	122.81	120.30
47	b4	5	A	C6-N1-C2	-5.01	115.59	118.60
42	HJ	639	ARG	CG-CD-NE	5.01	122.31	111.80
40	Bk	261	MET	CA-CB-CG	5.00	121.81	113.30
1	B0	165	ARG	CD-NE-CZ	5.00	130.60	123.60
41	Bl	20	LYS	CA-CB-CG	5.00	124.41	113.40
47	b4	27	U	N1-C2-N3	-5.00	111.90	114.90

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	BE	931	TYR	Sidechain
42	HJ	745	ARG	Sidechain
52	bH	1	U	Sidechain
62	bS	18	U	Sidechain
62	bS	21	U	Sidechain
62	bS	22	U	Sidechain
62	bS	5	U	Sidechain
63	bT	51	A	Sidechain
63	bT	52	A	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B0	2311	0	2283	6	0
2	B1	68	0	3	0	0
3	B2	2790	0	2770	12	0
4	B3	1735	0	1758	3	0
5	B4	663	0	684	3	0
6	B5	1109	0	1144	7	0
7	B6	943	0	963	2	0
8	B7	48	0	2	0	0
9	B8	84	0	2	0	0
9	Bj	84	0	3	0	0
10	B9	531	0	533	1	0
11	BA	4093	0	4060	11	0
12	BB	4313	0	4430	15	0
13	BC	1581	0	1643	4	0
14	BD	2682	0	2667	13	0
15	BE	5085	0	5150	47	0
16	BF	2195	0	2198	14	0
17	BG	1187	0	1220	4	0
18	BH	998	0	1050	3	0
19	BI	52	0	3	0	0
19	BN	52	0	2	0	0
19	BX	52	0	3	0	0
20	BJ	104	0	3	0	0
21	BK	1673	0	1689	5	0
22	BL	887	0	901	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	BO	2150	0	2220	8	0
24	BP	188	0	3	0	0
25	BQ	3588	0	3626	15	0
26	BS	1305	0	1320	6	0
27	BT	801	0	804	14	0
28	BU	56	0	2	0	0
29	BV	2181	0	2158	3	0
30	BW	2716	0	2681	22	0
31	BY	44	0	4	3	0
32	Ba	40	0	3	0	0
33	Bb	32	0	2	0	0
34	Bc	4276	0	4207	0	0
35	Bd	132	0	5	0	0
36	Be	72	0	2	0	0
37	Bg	1543	0	1534	0	0
38	Bh	1242	0	1259	0	0
39	Bi	928	0	936	0	0
40	Bk	3394	0	3540	0	0
41	Bl	1660	0	1739	0	0
42	HJ	2916	0	2948	16	0
43	HS	720	0	753	1	0
44	b1	160	0	81	0	0
45	b2	632	0	325	0	0
46	b3	100	0	51	0	0
47	b4	585	0	254	0	0
48	bA	571	0	286	0	0
49	bD	546	0	263	0	0
50	bE	1965	0	990	0	0
51	bG	80	0	41	0	0
52	bH	40	0	21	0	0
53	bI	60	0	31	0	0
54	bJ	1220	0	614	0	0
55	bK	1397	0	665	0	0
56	bL	1019	0	493	0	0
57	bN	1069	0	510	0	0
58	bO	2451	0	1152	0	0
59	bP	300	0	151	0	0
60	bQ	280	0	141	0	0
61	bR	408	0	202	0	0
62	bS	620	0	311	0	0
63	bT	1128	0	564	0	0
64	bU	500	0	251	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
65	bV	120	0	61	0	0
66	bY	220	0	111	0	0
All	All	80775	0	72479	212	0

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

All (212) 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)
27:BT:45:ARG:HG3	27:BT:51:HIS:CE1	1.46	1.50
27:BT:45:ARG:CG	27:BT:51:HIS:CE1	2.26	1.17
15:BE:971:THR:HG22	15:BE:1010:VAL:CG2	1.81	1.11
15:BE:971:THR:CG2	15:BE:1010:VAL:CG2	2.32	1.07
14:BD:246:LEU:HD12	14:BD:246:LEU:O	1.60	1.00
25:BQ:144:HIS:HB3	25:BQ:176:ASN:OD1	1.65	0.95
27:BT:45:ARG:HG3	27:BT:51:HIS:HE1	1.14	0.89
42:HJ:773:LEU:HG	42:HJ:774:VAL:H	1.39	0.86
15:BE:982:PHE:CZ	15:BE:984:GLU:OE1	2.31	0.83
15:BE:971:THR:HG22	15:BE:1010:VAL:HG21	1.61	0.83
11:BA:336:GLU:O	11:BA:340:SER:OG	2.00	0.80
6:B5:60:TYR:OH	15:BE:1043:LYS:HD2	1.80	0.80
15:BE:971:THR:HG22	15:BE:1010:VAL:HG22	1.63	0.79
25:BQ:144:HIS:CB	25:BQ:176:ASN:OD1	2.29	0.79
15:BE:971:THR:CG2	15:BE:1010:VAL:HG23	2.11	0.78
6:B5:60:TYR:OH	15:BE:1043:LYS:CD	2.32	0.78
15:BE:971:THR:CG2	15:BE:1010:VAL:HG21	2.13	0.74
17:BG:143:LEU:HD23	17:BG:147:GLU:OE2	1.86	0.74
15:BE:971:THR:HG21	15:BE:1010:VAL:CG2	2.16	0.74
15:BE:936:TRP:CZ3	15:BE:937:LEU:HD21	2.22	0.74
27:BT:45:ARG:CD	27:BT:51:HIS:ND1	2.49	0.73
6:B5:102:GLN:HE22	15:BE:1037:ALA:HB2	1.52	0.73
23:BO:41:SER:HA	23:BO:48:ARG:NH1	2.04	0.73
27:BT:45:ARG:CG	27:BT:51:HIS:ND1	2.51	0.73
23:BO:212:TRP:O	23:BO:214:LEU:HD12	1.89	0.72
14:BD:471:SER:O	14:BD:475:SER:OG	2.08	0.72
14:BD:304:CYS:SG	14:BD:305:TYR:N	2.63	0.71
13:BC:43:ARG:O	13:BC:46:LEU:HG	1.89	0.71
30:BW:70:ARG:NH2	30:BW:135:GLU:OE1	2.25	0.69
15:BE:798:ASP:OD2	15:BE:800:SER:OG	2.09	0.69
15:BE:971:THR:HG21	15:BE:1010:VAL:HG23	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:BA:465:LEU:HD23	11:BA:540:MET:CE	2.23	0.69
21:BK:19:ARG:O	42:HJ:648:ARG:NH2	2.26	0.68
30:BW:309:ALA:O	30:BW:312:THR:HG22	1.93	0.68
27:BT:45:ARG:HD3	27:BT:51:HIS:ND1	2.09	0.68
30:BW:303:PHE:CZ	30:BW:312:THR:HG21	2.28	0.68
15:BE:723:GLN:OE1	15:BE:727:ARG:NH1	2.27	0.68
42:HJ:773:LEU:HG	42:HJ:774:VAL:N	2.09	0.66
15:BE:982:PHE:CE2	15:BE:984:GLU:OE1	2.49	0.66
27:BT:45:ARG:HA	27:BT:51:HIS:HE1	1.62	0.64
25:BQ:144:HIS:HB3	25:BQ:176:ASN:CG	2.19	0.64
15:BE:323:SER:O	15:BE:327:ARG:NE	2.31	0.63
16:BF:137:SER:OG	16:BF:174:GLN:OE1	2.13	0.63
5:B4:108:PHE:O	5:B4:116:TYR:OH	2.16	0.63
27:BT:45:ARG:CG	27:BT:51:HIS:HE1	1.92	0.62
15:BE:421:LEU:HD23	15:BE:461:ARG:HG2	1.79	0.62
30:BW:343:GLU:HG2	30:BW:344:ASP:N	2.15	0.62
13:BC:90:LEU:O	13:BC:94:VAL:HG23	1.99	0.61
30:BW:343:GLU:HG2	30:BW:344:ASP:H	1.64	0.61
16:BF:74:LEU:HD11	16:BF:77:HIS:CD2	2.35	0.61
23:BO:212:TRP:O	23:BO:214:LEU:CD1	2.47	0.61
27:BT:45:ARG:CB	27:BT:51:HIS:CE1	2.83	0.61
15:BE:975:ARG:HD3	15:BE:1012:GLN:OE1	2.01	0.61
14:BD:223:THR:HG1	14:BD:228:SER:HG	1.49	0.60
21:BK:2:ASN:ND2	42:HJ:780:TRP:O	2.35	0.60
27:BT:47:ASP:O	30:BW:317:GLN:NE2	2.36	0.59
15:BE:860:MET:SD	15:BE:902:PHE:CE2	2.97	0.58
30:BW:199:CYS:SG	30:BW:200:ARG:N	2.76	0.58
15:BE:936:TRP:HZ3	15:BE:937:LEU:HD21	1.68	0.58
23:BO:41:SER:HA	23:BO:48:ARG:HH11	1.68	0.57
25:BQ:144:HIS:CG	25:BQ:176:ASN:OD1	2.57	0.57
12:BB:843:LEU:HD12	12:BB:846:GLN:HE21	1.68	0.57
27:BT:45:ARG:CD	27:BT:51:HIS:CE1	2.86	0.57
30:BW:78:CYS:SG	30:BW:79:LEU:N	2.78	0.56
11:BA:465:LEU:HD23	11:BA:540:MET:HE1	1.87	0.56
16:BF:262:PHE:O	16:BF:266:MET:HG2	2.06	0.56
3:B2:81:ARG:NH2	4:B3:89:TRP:O	2.38	0.56
11:BA:488:PRO:O	11:BA:490:HIS:CD2	2.58	0.56
42:HJ:773:LEU:CG	42:HJ:774:VAL:H	2.15	0.55
21:BK:135:GLU:OE1	21:BK:137:ARG:NH1	2.39	0.55
30:BW:309:ALA:O	30:BW:312:THR:CG2	2.55	0.54
21:BK:13:PHE:O	21:BK:19:ARG:NH1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B0:284:ARG:NH2	1:B0:287:GLU:OE2	2.41	0.54
6:B5:60:TYR:OH	15:BE:1043:LYS:CG	2.56	0.54
42:HJ:8:ARG:O	42:HJ:12:ARG:NH2	2.40	0.54
23:BO:212:TRP:N	23:BO:214:LEU:HD13	2.23	0.54
6:B5:102:GLN:HE22	15:BE:1037:ALA:CB	2.20	0.53
14:BD:267:ARG:HG2	14:BD:267:ARG:O	2.09	0.53
3:B2:320:GLU:OE1	3:B2:328:ARG:NH2	2.42	0.53
14:BD:246:LEU:O	14:BD:246:LEU:CD1	2.47	0.53
15:BE:860:MET:SD	15:BE:902:PHE:CD2	3.02	0.53
42:HJ:856:VAL:O	42:HJ:859:THR:OG1	2.26	0.53
5:B4:16:VAL:HG21	26:BS:77:LEU:HD13	1.90	0.53
11:BA:264:ASP:OD1	11:BA:265:SER:N	2.41	0.53
29:BV:255:CYS:C	30:BW:180:ASP:OD1	2.47	0.53
12:BB:1132:CYS:SG	12:BB:1133:GLN:N	2.83	0.52
1:B0:204:ILE:O	1:B0:208:GLY:N	2.42	0.52
15:BE:421:LEU:HG	15:BE:421:LEU:O	2.09	0.52
15:BE:613:ASN:OD1	15:BE:841:ARG:NH1	2.42	0.52
15:BE:346:GLU:O	15:BE:349:TRP:NE1	2.43	0.51
30:BW:115:CYS:SG	30:BW:116:ASP:N	2.83	0.51
13:BC:196:PHE:CE2	25:BQ:203:GLU:HG3	2.46	0.51
1:B0:155:SER:OG	25:BQ:357:ASP:OD1	2.16	0.51
14:BD:24:LEU:O	14:BD:29:TRP:NE1	2.44	0.51
15:BE:290:ARG:NH2	15:BE:347:GLU:OE1	2.44	0.51
16:BF:237:LEU:HD21	42:HJ:605:GLU:OE2	2.11	0.50
42:HJ:775:ALA:HB3	42:HJ:776:PRO:HD3	1.93	0.50
12:BB:1011:ALA:O	12:BB:1014:LYS:NZ	2.30	0.50
25:BQ:144:HIS:ND1	25:BQ:176:ASN:OD1	2.44	0.50
22:BL:75:ASP:OD1	22:BL:101:GLU:N	2.45	0.50
13:BC:44:TYR:OH	16:BF:38:THR:OG1	2.27	0.50
30:BW:343:GLU:CG	30:BW:344:ASP:H	2.25	0.50
16:BF:118:CYS:SG	16:BF:119:SER:N	2.85	0.50
15:BE:792:THR:O	15:BE:795:ARG:NH1	2.45	0.49
14:BD:91:ASN:O	14:BD:93:ARG:NH1	2.45	0.49
18:BH:75:ASP:N	18:BH:75:ASP:OD1	2.44	0.49
23:BO:213:ASN:C	23:BO:214:LEU:HD12	2.33	0.49
3:B2:91:ARG:O	4:B3:201:GLN:NE2	2.46	0.49
16:BF:240:ASP:O	42:HJ:617:ARG:NH2	2.45	0.49
25:BQ:508:ASN:OD1	25:BQ:512:GLN:N	2.46	0.49
14:BD:188:PRO:O	14:BD:191:VAL:HG22	2.12	0.49
15:BE:290:ARG:NH1	15:BE:301:PRO:O	2.44	0.49
16:BF:90:VAL:N	16:BF:91:PRO:CD	2.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:HJ:604:ARG:O	42:HJ:607:VAL:N	2.42	0.49
25:BQ:187:VAL:HG12	25:BQ:334:TYR:HE1	1.78	0.48
1:B0:256:LEU:O	1:B0:260:VAL:HG23	2.12	0.48
25:BQ:185:VAL:HG13	25:BQ:290:THR:CG2	2.42	0.48
26:BS:82:ASP:OD1	26:BS:82:ASP:N	2.46	0.48
15:BE:356:LEU:O	15:BE:358:ALA:N	2.47	0.48
15:BE:513:SER:O	15:BE:516:THR:OG1	2.31	0.48
26:BS:46:ARG:NH2	26:BS:50:GLU:OE2	2.46	0.48
15:BE:573:TYR:OH	15:BE:792:THR:N	2.47	0.48
12:BB:248:SER:O	12:BB:254:ASN:ND2	2.45	0.47
31:BY:8:UNK:C	31:BY:9:UNK:O	2.61	0.47
27:BT:45:ARG:CA	27:BT:51:HIS:HE1	2.26	0.47
3:B2:35:ASP:OD2	3:B2:317:GLN:NE2	2.46	0.47
3:B2:267:ASP:O	3:B2:270:THR:OG1	2.33	0.47
16:BF:43:THR:OG1	16:BF:60:ARG:O	2.19	0.47
30:BW:345:ASP:N	30:BW:345:ASP:OD1	2.48	0.47
15:BE:580:THR:OG1	15:BE:583:GLU:OE1	2.33	0.47
16:BF:123:ARG:O	16:BF:126:VAL:HG12	2.15	0.47
30:BW:343:GLU:CG	30:BW:344:ASP:N	2.79	0.46
31:BY:8:UNK:O	31:BY:9:UNK:C	2.63	0.46
16:BF:240:ASP:OD2	42:HJ:665:ARG:NH1	2.49	0.46
16:BF:238:VAL:O	42:HJ:618:GLN:NE2	2.47	0.45
14:BD:381:LEU:HD22	14:BD:431:TRP:CE2	2.52	0.45
16:BF:74:LEU:HD13	16:BF:76:HIS:CE1	2.51	0.45
25:BQ:35:SER:N	25:BQ:36:PRO:CD	2.80	0.45
15:BE:636:ARG:NH2	15:BE:739:ASP:OD1	2.49	0.45
21:BK:7:LEU:O	21:BK:7:LEU:HD23	2.16	0.45
30:BW:127:PHE:O	30:BW:186:ARG:NH1	2.49	0.45
18:BH:96:MET:HE3	18:BH:115:GLY:HA3	1.98	0.45
25:BQ:56:ALA:O	25:BQ:60:THR:OG1	2.29	0.45
26:BS:107:LEU:HD23	26:BS:107:LEU:O	2.17	0.45
27:BT:62:ARG:NH1	27:BT:79:ARG:O	2.50	0.45
6:B5:60:TYR:OH	15:BE:1043:LYS:HG2	2.16	0.45
12:BB:679:LEU:HD23	12:BB:679:LEU:O	2.17	0.45
25:BQ:143:VAL:HG12	25:BQ:143:VAL:O	2.17	0.44
3:B2:122:GLU:O	3:B2:122:GLU:HG2	2.16	0.44
25:BQ:139:GLU:O	25:BQ:140:ILE:HG23	2.17	0.44
30:BW:217:VAL:O	30:BW:217:VAL:HG22	2.16	0.44
15:BE:476:VAL:HG12	15:BE:476:VAL:O	2.17	0.44
15:BE:792:THR:OG1	15:BE:795:ARG:NH2	2.44	0.44
4:B3:4:VAL:O	10:B9:59:ARG:NH1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B5:60:TYR:CZ	15:BE:1043:LYS:HE3	2.52	0.43
29:BV:125:SER:OG	29:BV:128:ASP:OD2	2.29	0.43
42:HJ:775:ALA:HB3	42:HJ:776:PRO:CD	2.47	0.43
17:BG:83:TYR:OH	42:HJ:604:ARG:NH1	2.51	0.43
26:BS:27:VAL:O	26:BS:31:THR:OG1	2.35	0.43
3:B2:240:ARG:O	7:B6:91:ARG:NH2	2.51	0.43
12:BB:422:GLU:HG2	12:BB:423:ILE:N	2.34	0.43
17:BG:24:HIS:O	17:BG:28:THR:OG1	2.30	0.43
18:BH:62:VAL:HG13	18:BH:63:ILE:HG13	1.99	0.43
3:B2:44:SER:O	3:B2:48:ARG:NH2	2.52	0.43
5:B4:27:GLN:OE1	5:B4:29:TRP:NE1	2.49	0.43
7:B6:100:ARG:NH2	11:BA:623:ASP:OD2	2.51	0.43
31:BY:8:UNK:O	31:BY:9:UNK:O	2.37	0.43
43:HS:224:GLU:O	43:HS:229:GLU:HB2	2.18	0.43
3:B2:5:SER:O	3:B2:10:GLN:NE2	2.52	0.43
14:BD:162:PHE:N	14:BD:163:PRO:CD	2.82	0.43
15:BE:958:LEU:HD23	15:BE:958:LEU:C	2.39	0.43
30:BW:190:VAL:HG22	30:BW:190:VAL:O	2.19	0.43
3:B2:46:ARG:O	3:B2:47:HIS:HB2	2.18	0.43
15:BE:913:LYS:HG2	15:BE:929:ASN:ND2	2.34	0.43
15:BE:971:THR:HG21	15:BE:1010:VAL:HG21	1.91	0.43
12:BB:169:LEU:O	12:BB:228:GLN:NE2	2.48	0.42
3:B2:158:ARG:NH2	3:B2:163:ALA:O	2.49	0.42
29:BV:255:CYS:O	30:BW:180:ASP:OD1	2.37	0.42
11:BA:465:LEU:CD2	11:BA:540:MET:CE	2.96	0.42
42:HJ:702:ILE:HG12	42:HJ:731:VAL:HG22	2.01	0.42
12:BB:988:SER:N	12:BB:989:PRO:CD	2.82	0.42
17:BG:144:LEU:O	17:BG:147:GLU:HG2	2.20	0.42
11:BA:217:LEU:HD23	11:BA:233:LYS:HZ3	1.85	0.41
12:BB:656:GLU:O	12:BB:659:VAL:HG22	2.20	0.41
11:BA:107:VAL:HG13	11:BA:117:VAL:HG22	2.02	0.41
15:BE:639:GLN:OE1	15:BE:639:GLN:HA	2.21	0.41
15:BE:786:SER:N	15:BE:787:PRO:CD	2.83	0.41
30:BW:90:LEU:O	30:BW:95:ARG:NH2	2.53	0.41
30:BW:185:PHE:HE2	30:BW:195:CYS:HG	1.68	0.41
15:BE:739:ASP:O	15:BE:804:ILE:HG22	2.21	0.41
15:BE:1038:ASN:OD1	26:BS:7:PHE:HD1	2.03	0.41
22:BL:44:ASP:OD1	22:BL:44:ASP:N	2.46	0.41
11:BA:234:ASN:O	11:BA:237:VAL:HG22	2.19	0.41
12:BB:964:VAL:O	14:BD:17:ARG:NH1	2.54	0.41
3:B2:206:HIS:O	3:B2:209:VAL:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:BA:564:THR:O	11:BA:564:THR:OG1	2.38	0.41
22:BL:33:ASP:N	22:BL:33:ASP:OD1	2.54	0.41
30:BW:358:ASP:OD1	30:BW:358:ASP:N	2.54	0.41
12:BB:174:THR:CG2	12:BB:175:PRO:HD3	2.51	0.41
12:BB:340:ALA:O	12:BB:342:GLU:N	2.50	0.41
14:BD:328:ASP:OD1	14:BD:331:ARG:NH2	2.54	0.41
23:BO:211:ALA:C	23:BO:214:LEU:HD13	2.41	0.41
12:BB:318:SER:N	12:BB:319:PRO:CD	2.85	0.40
15:BE:1002:MET:HG3	15:BE:1006:ASP:HB3	2.03	0.40
27:BT:45:ARG:CB	27:BT:51:HIS:HE1	2.29	0.40
1:B0:230:ARG:NH1	16:BF:51:SER:O	2.55	0.40
25:BQ:360:ASP:OD1	25:BQ:360:ASP:N	2.51	0.40
30:BW:117:ARG:NH2	30:BW:119:ASP:OD2	2.54	0.40
1:B0:211:LEU:O	1:B0:214:VAL:HG12	2.21	0.40
12:BB:173:THR:HG23	12:BB:175:PRO:HD2	2.04	0.40
23:BO:80:THR:HA	23:BO:85:VAL:HG11	2.02	0.40
12:BB:27:PRO:O	12:BB:28:TYR:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B0	274/680 (40%)	259 (94%)	15 (6%)	0	100	100
3	B2	333/738 (45%)	321 (96%)	12 (4%)	0	100	100
4	B3	212/377 (56%)	208 (98%)	4 (2%)	0	100	100
5	B4	76/138 (55%)	75 (99%)	1 (1%)	0	100	100
6	B5	138/393 (35%)	133 (96%)	5 (4%)	0	100	100
7	B6	111/163 (68%)	105 (95%)	6 (5%)	0	100	100
10	B9	60/233 (26%)	60 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	BA	516/939 (55%)	503 (98%)	13 (2%)	0	100	100
12	BB	518/1547 (34%)	490 (95%)	28 (5%)	0	100	100
13	BC	196/421 (47%)	191 (97%)	5 (3%)	0	100	100
14	BD	331/686 (48%)	312 (94%)	19 (6%)	0	100	100
15	BE	612/1053 (58%)	580 (95%)	30 (5%)	2 (0%)	37	66
16	BF	267/304 (88%)	262 (98%)	5 (2%)	0	100	100
17	BG	146/160 (91%)	141 (97%)	5 (3%)	0	100	100
18	BH	123/129 (95%)	122 (99%)	1 (1%)	0	100	100
21	BK	196/530 (37%)	190 (97%)	6 (3%)	0	100	100
22	BL	101/116 (87%)	101 (100%)	0	0	100	100
23	BO	255/395 (65%)	248 (97%)	7 (3%)	0	100	100
25	BQ	447/698 (64%)	433 (97%)	14 (3%)	0	100	100
26	BS	152/243 (63%)	144 (95%)	8 (5%)	0	100	100
27	BT	98/280 (35%)	88 (90%)	10 (10%)	0	100	100
29	BV	260/597 (44%)	248 (95%)	12 (5%)	0	100	100
30	BW	335/547 (61%)	307 (92%)	28 (8%)	0	100	100
34	Bc	535/716 (75%)	522 (98%)	13 (2%)	0	100	100
37	Bg	183/302 (61%)	164 (90%)	18 (10%)	1 (0%)	25	56
38	Bh	151/167 (90%)	149 (99%)	2 (1%)	0	100	100
39	Bi	111/268 (41%)	109 (98%)	2 (2%)	0	100	100
40	Bk	413/447 (92%)	404 (98%)	9 (2%)	0	100	100
41	Bl	198/593 (33%)	184 (93%)	14 (7%)	0	100	100
42	HJ	349/1140 (31%)	325 (93%)	24 (7%)	0	100	100
43	HS	86/235 (37%)	83 (96%)	3 (4%)	0	100	100
All	All	7783/15235 (51%)	7461 (96%)	319 (4%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	BE	915	PRO
37	Bg	202	PRO
15	BE	935	PRO

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	B0	238/558 (43%)	234 (98%)	4 (2%)	56	74
3	B2	297/648 (46%)	293 (99%)	4 (1%)	65	79
4	B3	177/302 (59%)	174 (98%)	3 (2%)	56	74
5	B4	72/123 (58%)	71 (99%)	1 (1%)	62	78
6	B5	114/328 (35%)	114 (100%)	0	100	100
7	B6	98/142 (69%)	98 (100%)	0	100	100
10	B9	55/197 (28%)	55 (100%)	0	100	100
11	BA	429/769 (56%)	421 (98%)	8 (2%)	52	72
12	BB	465/1261 (37%)	459 (99%)	6 (1%)	65	79
13	BC	166/351 (47%)	166 (100%)	0	100	100
14	BD	276/548 (50%)	273 (99%)	3 (1%)	70	82
15	BE	541/908 (60%)	539 (100%)	2 (0%)	89	93
16	BF	227/252 (90%)	227 (100%)	0	100	100
17	BG	134/145 (92%)	134 (100%)	0	100	100
18	BH	109/115 (95%)	109 (100%)	0	100	100
21	BK	183/456 (40%)	182 (100%)	1 (0%)	86	91
22	BL	94/106 (89%)	94 (100%)	0	100	100
23	BO	230/346 (66%)	229 (100%)	1 (0%)	89	93
25	BQ	376/572 (66%)	373 (99%)	3 (1%)	79	87
26	BS	137/207 (66%)	134 (98%)	3 (2%)	47	69
27	BT	86/249 (34%)	84 (98%)	2 (2%)	45	68
29	BV	238/525 (45%)	237 (100%)	1 (0%)	89	93
30	BW	296/475 (62%)	292 (99%)	4 (1%)	62	78
34	Bc	458/620 (74%)	454 (99%)	4 (1%)	75	85
37	Bg	160/251 (64%)	158 (99%)	2 (1%)	65	79
38	Bh	130/143 (91%)	129 (99%)	1 (1%)	79	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	Bi	99/221 (45%)	98 (99%)	1 (1%)	73	84
40	Bk	360/385 (94%)	360 (100%)	0	100	100
41	Bl	181/534 (34%)	181 (100%)	0	100	100
42	HJ	307/968 (32%)	305 (99%)	2 (1%)	81	88
43	HS	78/207 (38%)	78 (100%)	0	100	100
All	All	6811/12912 (53%)	6755 (99%)	56 (1%)	77	87

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B0	173	ARG
1	B0	248	TRP
1	B0	284	ARG
1	B0	294	ARG
3	B2	79	PHE
3	B2	169	PHE
3	B2	219	ARG
3	B2	246	TYR
4	B3	16	ARG
4	B3	89	TRP
4	B3	214	ARG
5	B4	17	PHE
11	BA	38	LEU
11	BA	97	PHE
11	BA	221	MET
11	BA	343	CYS
11	BA	357	HIS
11	BA	384	ARG
11	BA	446	ARG
11	BA	531	TRP
12	BB	151	HIS
12	BB	250	PHE
12	BB	253	ARG
12	BB	944	ASP
12	BB	992	LYS
12	BB	1014	LYS
14	BD	265	ARG
14	BD	431	TRP
14	BD	452	ARG
15	BE	304	ARG

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Mol	Chain	Res	Type
15	BE	464	ASP
21	BK	15	TYR
23	BO	36	HIS
25	BQ	333	LEU
25	BQ	334	TYR
25	BQ	433	LYS
26	BS	61	ARG
26	BS	96	ARG
26	BS	233	PHE
27	BT	17	LYS
27	BT	99	ARG
29	BV	152	ARG
30	BW	96	LYS
30	BW	258	PHE
30	BW	276	TYR
30	BW	287	LYS
34	Bc	1	ARG
34	Bc	93	PHE
34	Bc	99	ASP
34	Bc	139	TYR
37	Bg	21	HIS
37	Bg	53	LYS
38	Bh	129	ARG
39	Bi	139	ARG
42	HJ	812	ARG
42	HJ	862	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
3	B2	176	HIS
6	B5	22	HIS
11	BA	490	HIS
12	BB	846	GLN
15	BE	929	ASN
16	BF	77	HIS
34	Bc	45	ASN
37	Bg	49	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
44	b1	7/8 (87%)	0	0
45	b2	29/48 (60%)	2 (6%)	0
46	b3	4/5 (80%)	2 (50%)	0
47	b4	26/34 (76%)	3 (11%)	0
48	bA	26/34 (76%)	2 (7%)	0
49	bD	24/27 (88%)	5 (20%)	0
50	bE	90/107 (84%)	22 (24%)	0
51	bG	3/4 (75%)	2 (66%)	0
52	bH	1/2 (50%)	1 (100%)	0
53	bI	2/3 (66%)	2 (100%)	0
54	bJ	57/71 (80%)	16 (28%)	0
55	bK	63/83 (75%)	12 (19%)	0
56	bL	47/48 (97%)	9 (19%)	0
57	bN	48/122 (39%)	7 (14%)	0
58	bO	114/115 (99%)	24 (21%)	0
59	bP	14/15 (93%)	1 (7%)	0
60	bQ	13/14 (92%)	3 (23%)	0
61	bR	18/31 (58%)	4 (22%)	0
62	bS	30/31 (96%)	11 (36%)	0
63	bT	51/60 (85%)	11 (21%)	0
64	bU	24/25 (96%)	6 (25%)	0
65	bV	5/6 (83%)	1 (20%)	0
66	bY	10/11 (90%)	2 (20%)	0
All	All	706/904 (78%)	148 (20%)	0

All (148) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
45	b2	31	A
45	b2	48	A
46	b3	4	U
46	b3	5	U
47	b4	2	G
47	b4	26	G
47	b4	27	U
48	bA	10	G
48	bA	27	A
49	bD	8	A
49	bD	9	A
49	bD	10	G
49	bD	11	G
49	bD	27	G
50	bE	20	G

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Mol	Chain	Res	Type
50	bE	21	G
50	bE	26	G
50	bE	40	G
50	bE	43	A
50	bE	47	C
50	bE	50	U
50	bE	51	G
50	bE	52	G
50	bE	53	A
50	bE	54	U
50	bE	55	U
50	bE	57	G
50	bE	58	A
50	bE	67	G
50	bE	73	U
50	bE	75	C
50	bE	81	U
50	bE	82	U
50	bE	84	A
50	bE	86	A
50	bE	87	A
51	bG	3	U
51	bG	4	U
52	bH	2	U
53	bI	2	U
53	bI	3	U
54	bJ	10	U
54	bJ	11	U
54	bJ	13	A
54	bJ	16	U
54	bJ	30	A
54	bJ	31	C
54	bJ	32	U
54	bJ	34	U
54	bJ	35	A
54	bJ	45	C
54	bJ	50	U
54	bJ	58	A
54	bJ	59	C
54	bJ	60	U
54	bJ	61	U
54	bJ	65	A

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Mol	Chain	Res	Type
55	bK	6	U
55	bK	8	C
55	bK	23	A
55	bK	31	U
55	bK	32	U
55	bK	34	U
55	bK	35	A
55	bK	42	A
55	bK	51	G
55	bK	52	A
55	bK	53	C
55	bK	61	A
56	bL	16	C
56	bL	25	U
56	bL	26	A
56	bL	28	G
56	bL	29	U
56	bL	30	C
56	bL	31	A
56	bL	32	A
56	bL	36	U
57	bN	10	G
57	bN	16	U
57	bN	29	G
57	bN	38	U
57	bN	39	A
57	bN	40	G
57	bN	49	U
58	bO	2	G
58	bO	3	A
58	bO	9	G
58	bO	16	C
58	bO	23	A
58	bO	24	A
58	bO	34	A
58	bO	36	A
58	bO	42	C
58	bO	56	U
58	bO	63	U
58	bO	65	G
58	bO	67	A
58	bO	68	G

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Mol	Chain	Res	Type
58	bO	69	A
58	bO	74	A
58	bO	75	G
58	bO	86	A
58	bO	88	A
58	bO	89	U
58	bO	91	C
58	bO	97	G
58	bO	100	A
58	bO	103	A
59	bP	15	U
60	bQ	6	U
60	bQ	7	U
60	bQ	14	U
61	bR	5	C
61	bR	6	A
61	bR	13	A
61	bR	14	U
62	bS	7	U
62	bS	13	U
62	bS	18	U
62	bS	19	U
62	bS	20	U
62	bS	21	U
62	bS	22	U
62	bS	23	U
62	bS	24	U
62	bS	25	U
62	bS	26	U
63	bT	15	A
63	bT	17	A
63	bT	19	G
63	bT	21	U
63	bT	22	A
63	bT	23	G
63	bT	32	G
63	bT	35	C
63	bT	44	G
63	bT	46	A
63	bT	50	A
64	bU	3	U
64	bU	12	U

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Mol	Chain	Res	Type
64	bU	18	U
64	bU	19	U
64	bU	22	U
64	bU	25	U
65	bV	6	U
66	bY	6	U
66	bY	9	U

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

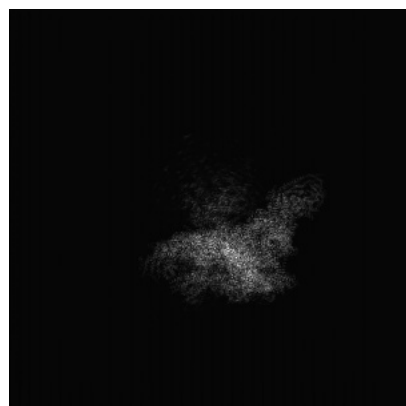
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50470. These allow visual inspection of the internal detail of the map and identification of artifacts.

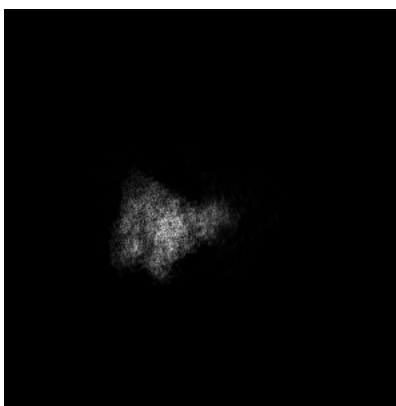
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

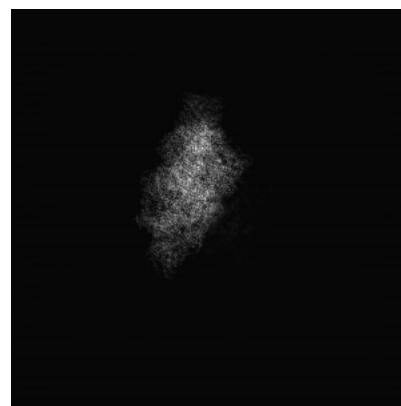
6.1.1 Primary map



X

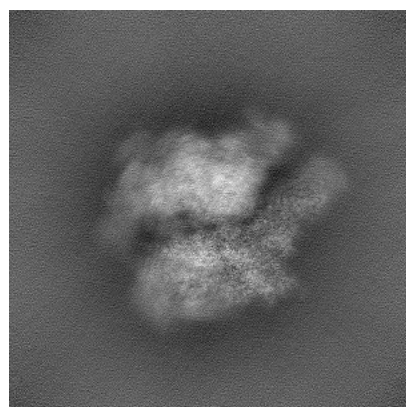


Y

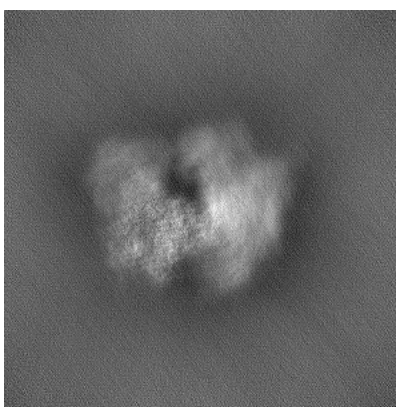


Z

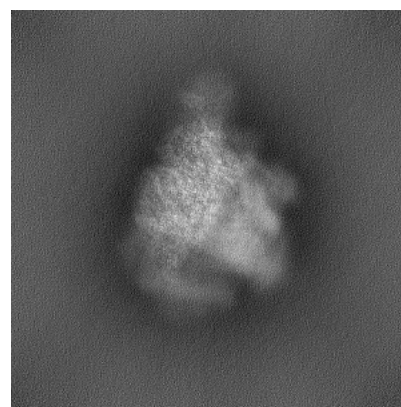
6.1.2 Raw map



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: 210

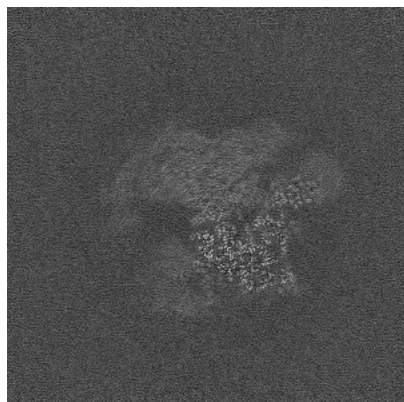


Y Index: 210

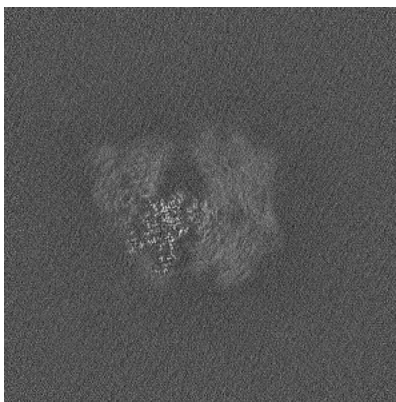


Z Index: 210

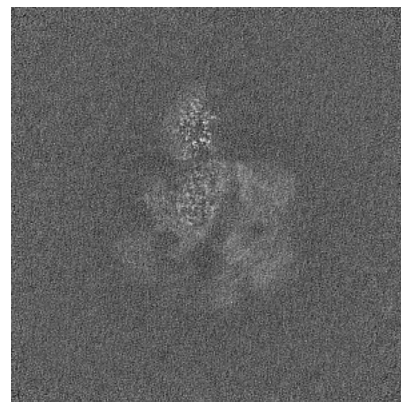
6.2.2 Raw map



X Index: 210



Y Index: 210



Z Index: 210

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: 196

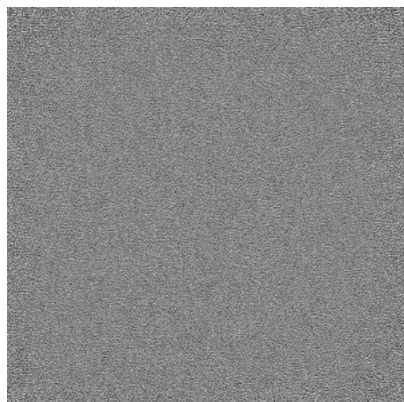


Y Index: 241

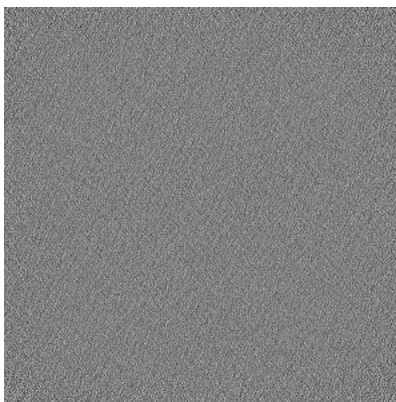


Z Index: 165

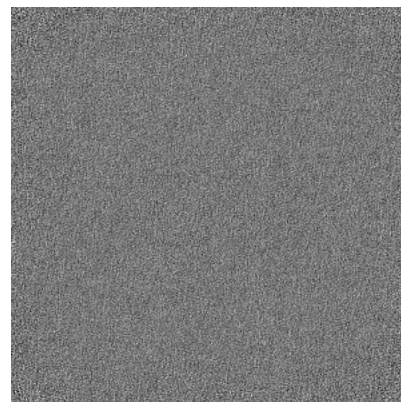
6.3.2 Raw map



X Index: 0



Y Index: 0

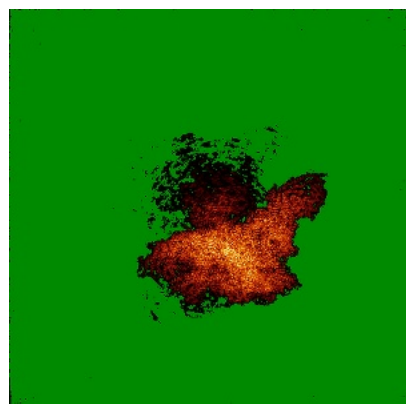


Z Index: 419

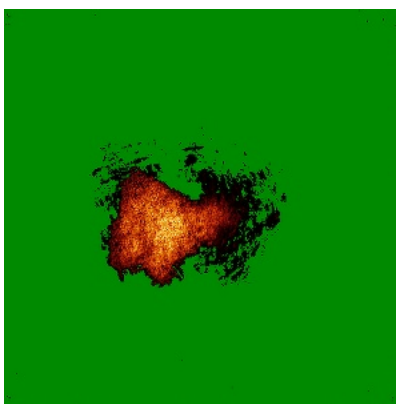
The images above show the largest variance slices of the map in three orthogonal directions.

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

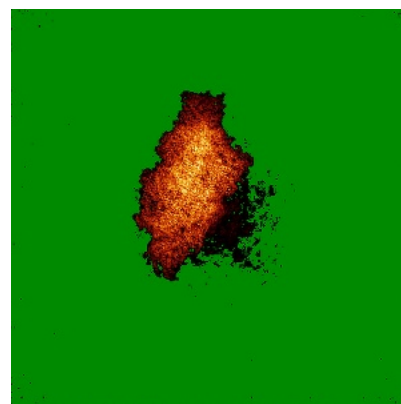
6.4.1 Primary map



X

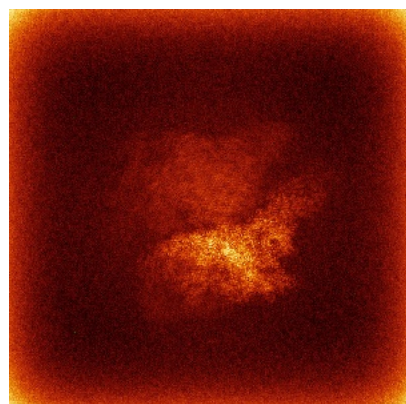


Y

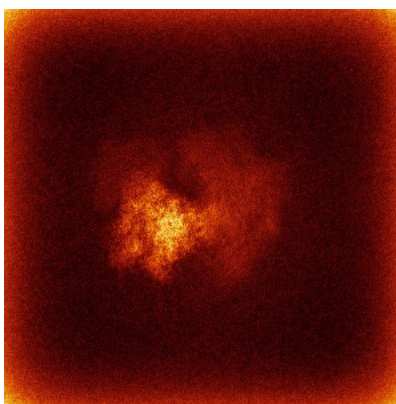


Z

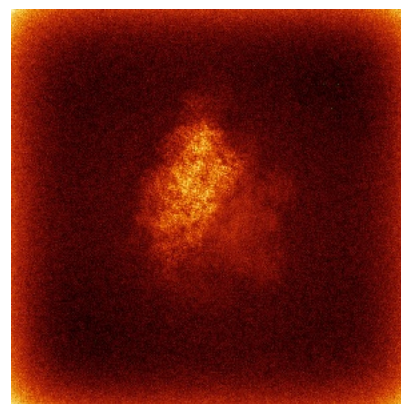
6.4.2 Raw map



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.

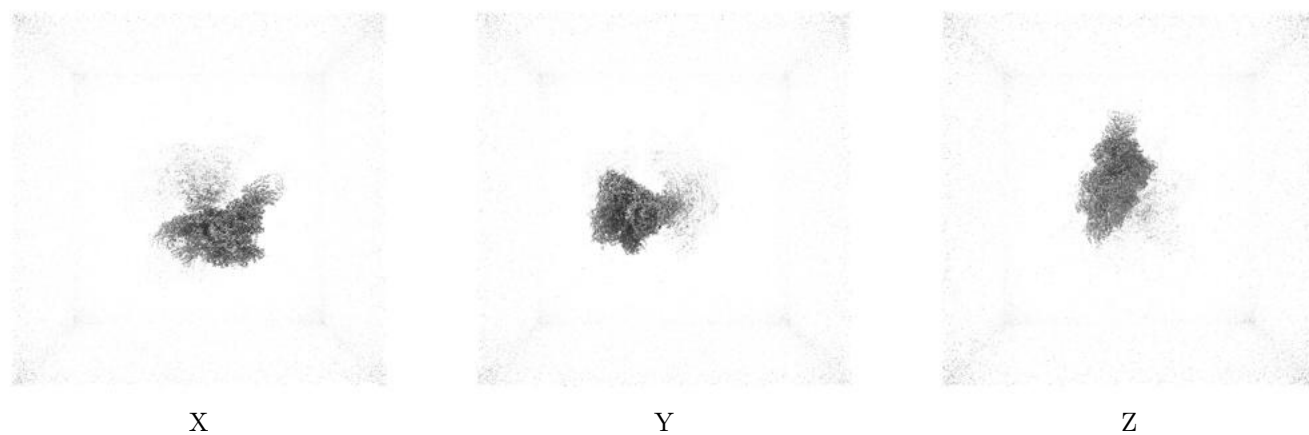
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

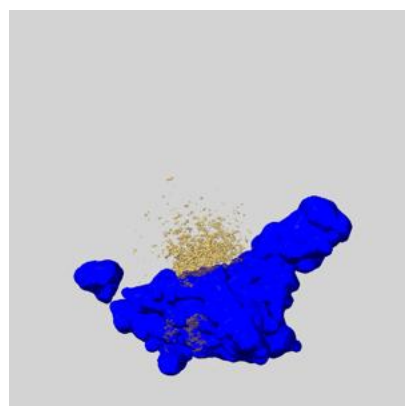
6.6 Mask visualisation [i](#)

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

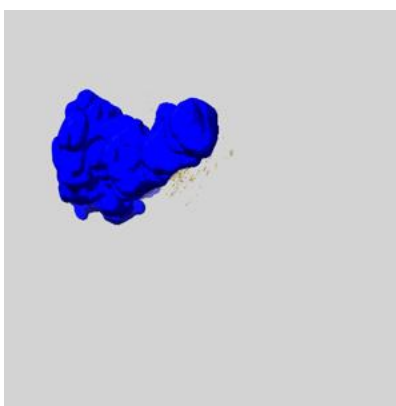
A mask typically either:

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

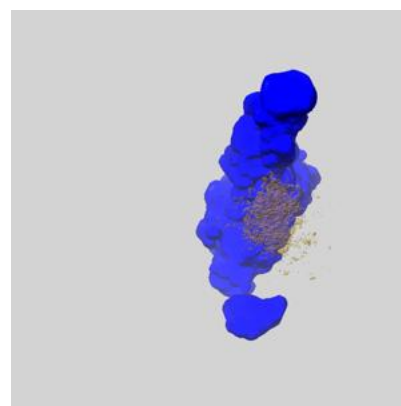
6.6.1 emd_50470_msk_1.map [i](#)



X



Y

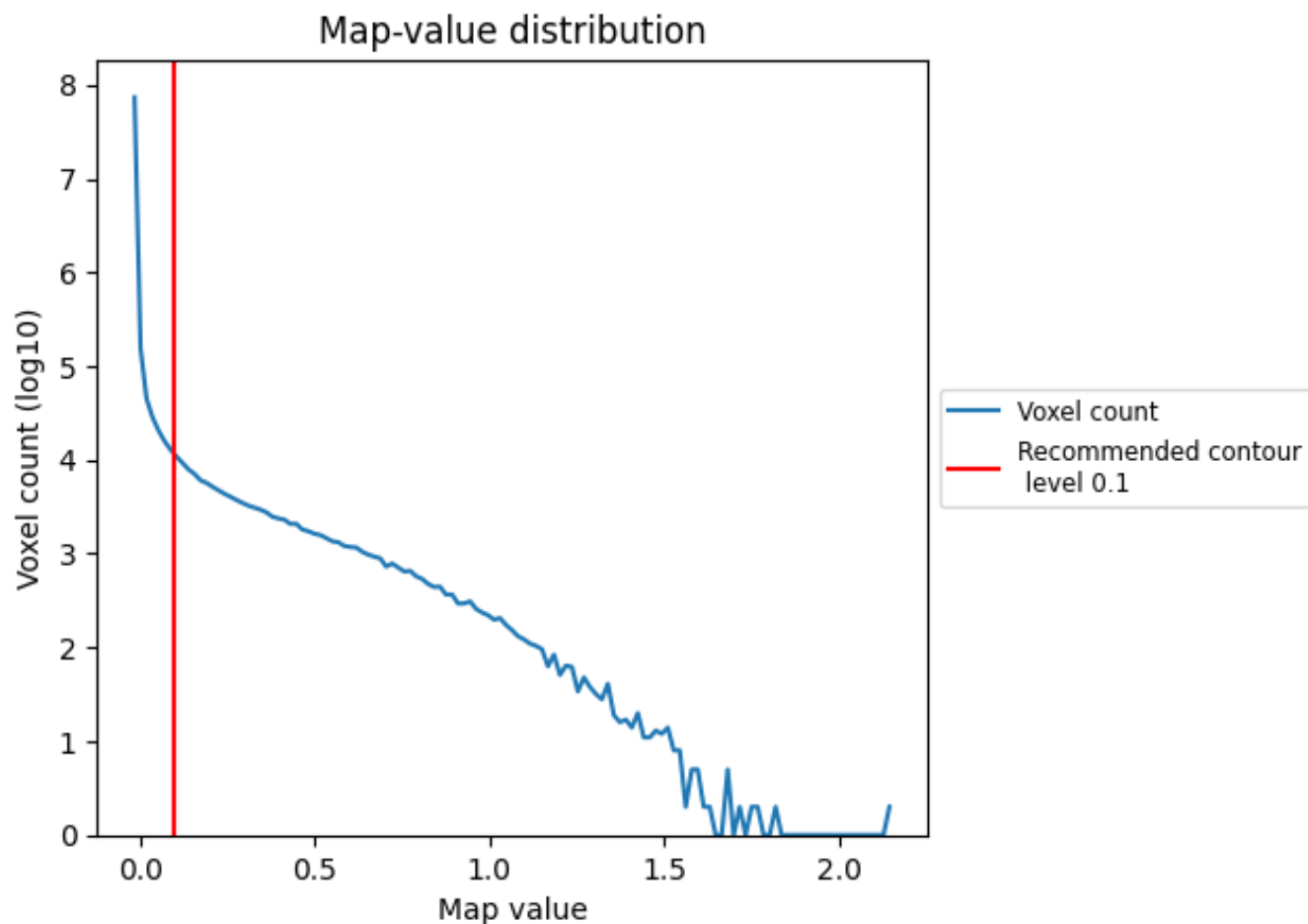


Z

7 Map analysis [i](#)

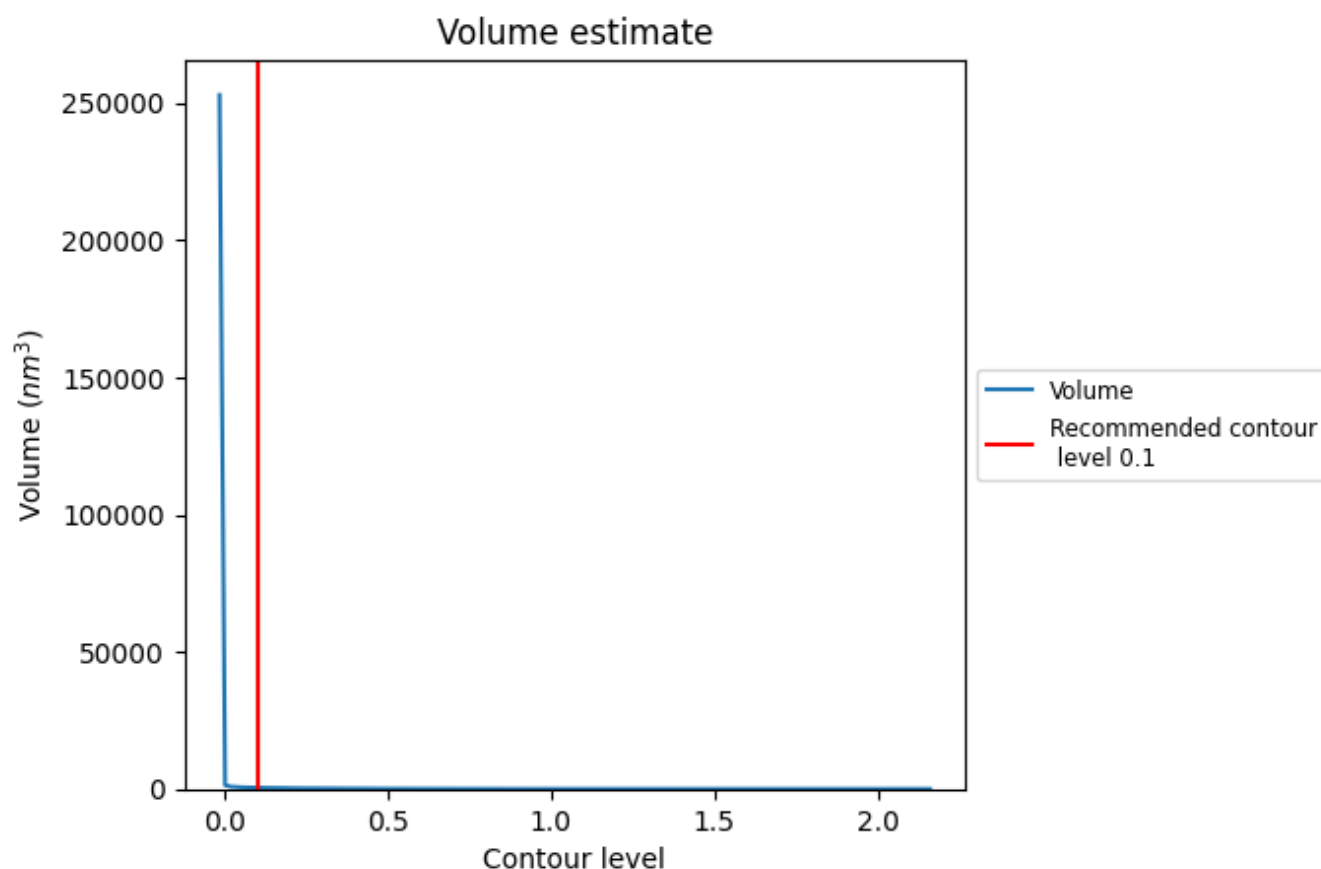
This section contains the results of statistical analysis of the map.

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.

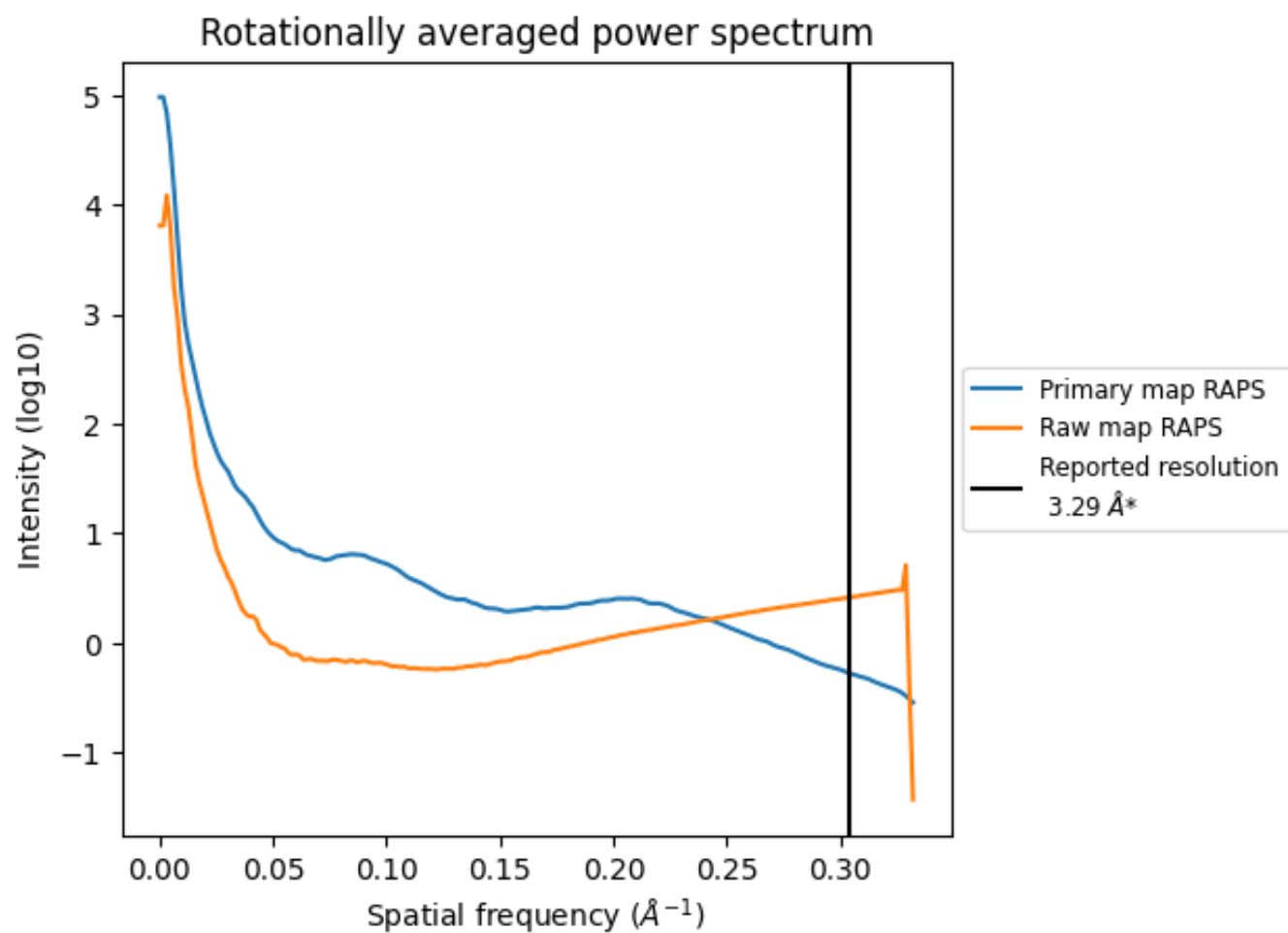
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 439 nm^3 ; this corresponds to an approximate mass of 397 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 ⓘ

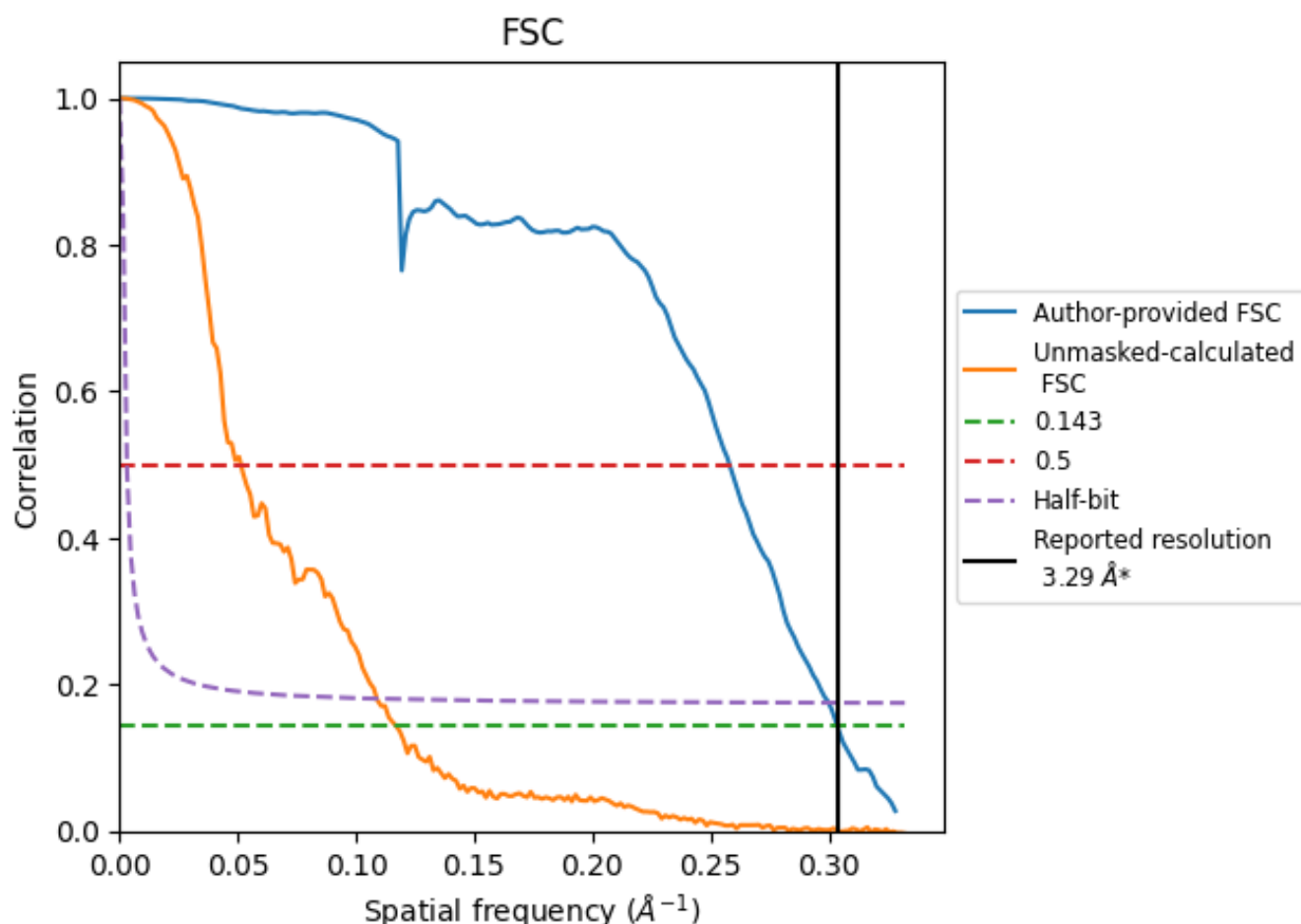


*Reported resolution corresponds to spatial frequency of 0.304 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.304 Å⁻¹

8.2 Resolution estimates [i](#)

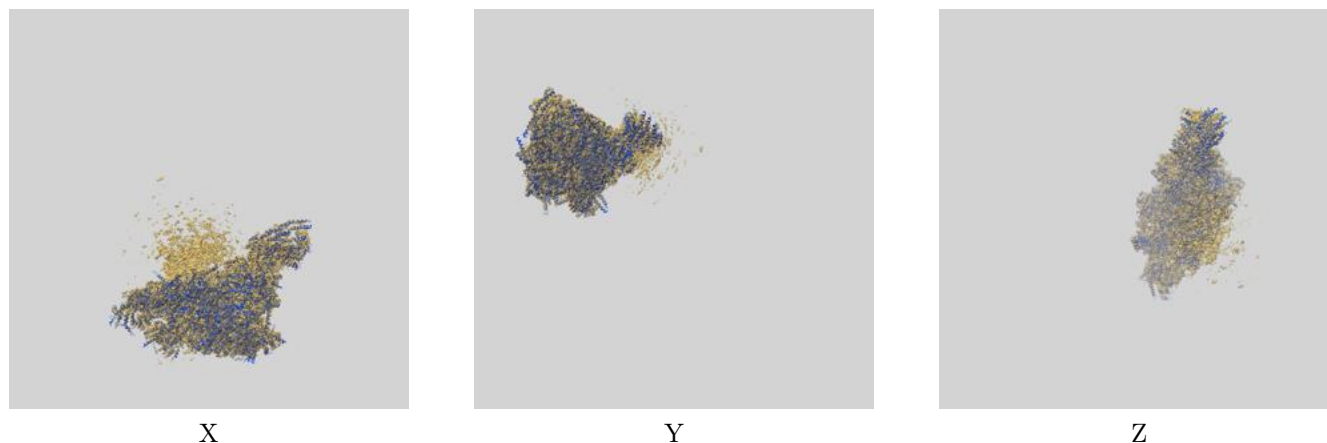
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.29	-	-
Author-provided FSC curve	3.29	3.88	3.33
Unmasked-calculated*	8.55	19.46	9.18

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.55 differs from the reported value 3.29 by more than 10 %

9 Map-model fit [i](#)

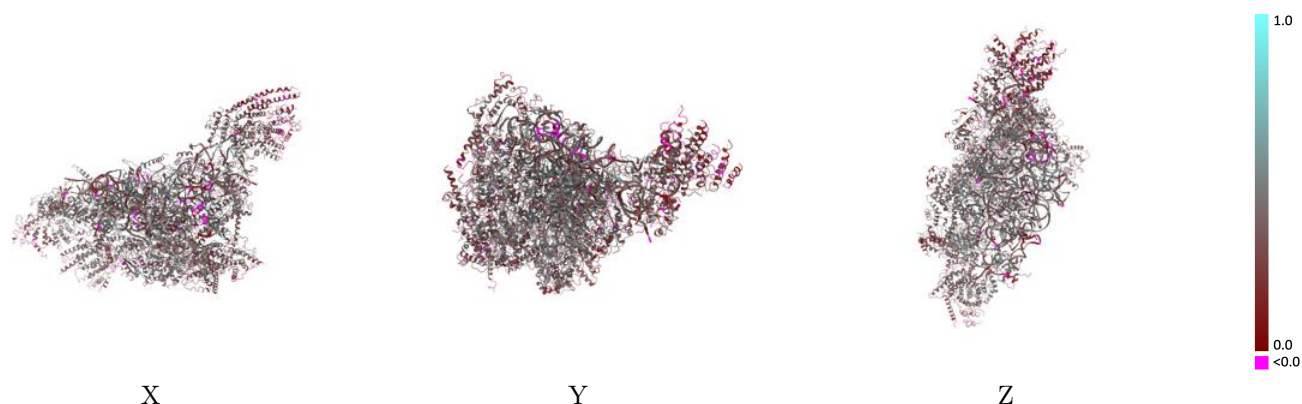
This section contains information regarding the fit between EMDB map EMD-50470 and PDB model 9FIA. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

9.1 Map-model overlay [i](#)



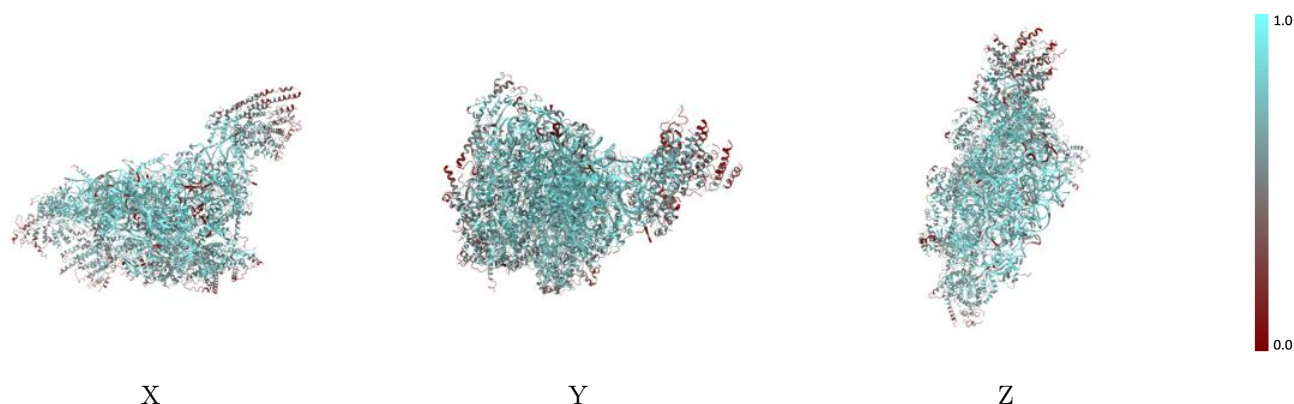
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



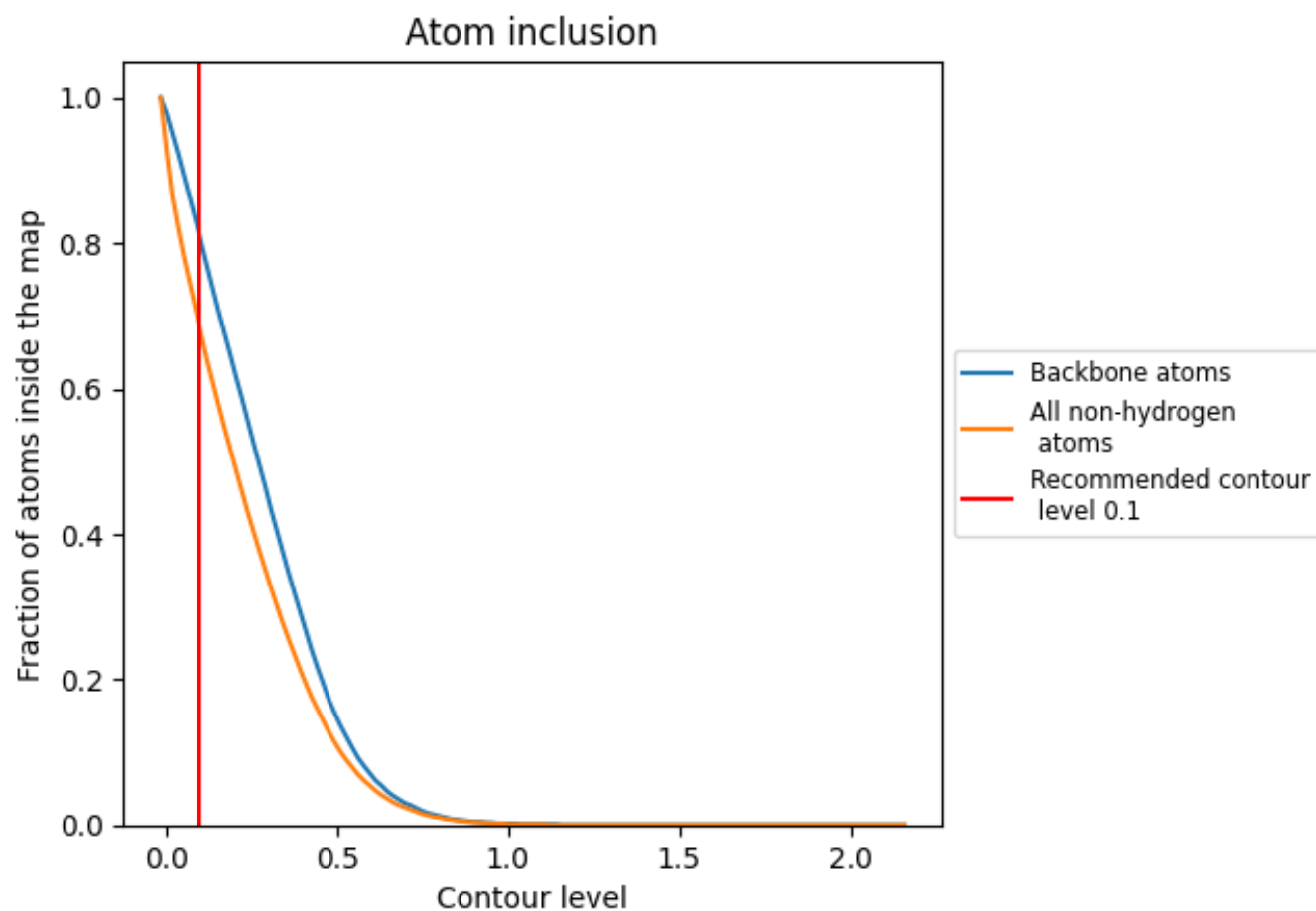
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 81% of all backbone atoms, 68% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6830	 0.3530
B0	 0.5680	 0.3020
B1	 0.7500	 0.4160
B2	 0.6760	 0.3560
B3	 0.7200	 0.3910
B4	 0.7010	 0.4030
B5	 0.7510	 0.3930
B6	 0.8290	 0.4550
B7	 0.2500	 0.2890
B8	 0.6550	 0.4170
B9	 0.7440	 0.3960
BA	 0.6590	 0.3660
BB	 0.5020	 0.2630
BC	 0.6700	 0.3640
BD	 0.5540	 0.2860
BE	 0.5270	 0.3000
BF	 0.6900	 0.3860
BG	 0.6830	 0.3790
BH	 0.8530	 0.4580
BI	 0.8460	 0.4210
BJ	 0.6250	 0.4180
BK	 0.8060	 0.4230
BL	 0.8630	 0.4570
BN	 0.6150	 0.3530
BO	 0.8030	 0.4380
BP	 0.8080	 0.4020
BQ	 0.7070	 0.3770
BS	 0.5640	 0.3120
BT	 0.7310	 0.3420
BU	 0.5890	 0.3880
BV	 0.6830	 0.3720
BW	 0.6510	 0.3050
BX	 0.7880	 0.5010
BY	 0.2270	 0.1740
Ba	 0.4000	 0.3490



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Chain	Atom inclusion	Q-score
Bb	 0.5940	 0.3650
Bc	 0.6780	 0.3710
Bd	 0.7880	 0.3780
Be	 0.7920	 0.4840
Bg	 0.7550	 0.3820
Bh	 0.7780	 0.4300
Bi	 0.7450	 0.4040
Bj	 0.9290	 0.5160
Bk	 0.6500	 0.3530
Bl	 0.6760	 0.3490
HJ	 0.6470	 0.3320
HS	 0.5180	 0.2740
b1	 0.8500	 0.3990
b2	 0.7780	 0.3900
b3	 0.5000	 0.2460
b4	 0.7280	 0.3060
bA	 0.7850	 0.3670
bD	 0.7970	 0.3800
bE	 0.7840	 0.3460
bG	 0.1630	 -0.1460
bH	 0.6500	 0.1360
bI	 0.1330	 -0.1050
bJ	 0.6640	 0.2890
bK	 0.6900	 0.3040
bL	 0.8390	 0.3670
bN	 0.7830	 0.3630
bO	 0.8280	 0.3940
bP	 0.7730	 0.3660
bQ	 0.7040	 0.3080
bR	 0.8140	 0.3820
bS	 0.7660	 0.3670
bT	 0.8130	 0.3740
bU	 0.7760	 0.3190
bV	 0.8830	 0.4030
bY	 0.7680	 0.3110