



Full wwPDB EM Validation Report ⓘ

Jun 24, 2026 – 05:33 PM EDT

PDB ID : 7UW1 / pdb_00007uw1
EMDB ID : EMD-26822
Title : A. baumannii 70S ribosome-Streptothricin-D complex
Authors : Morgan, C.E.; Yu, E.W.
Deposited on : 2022-05-02
Resolution : 2.21 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:

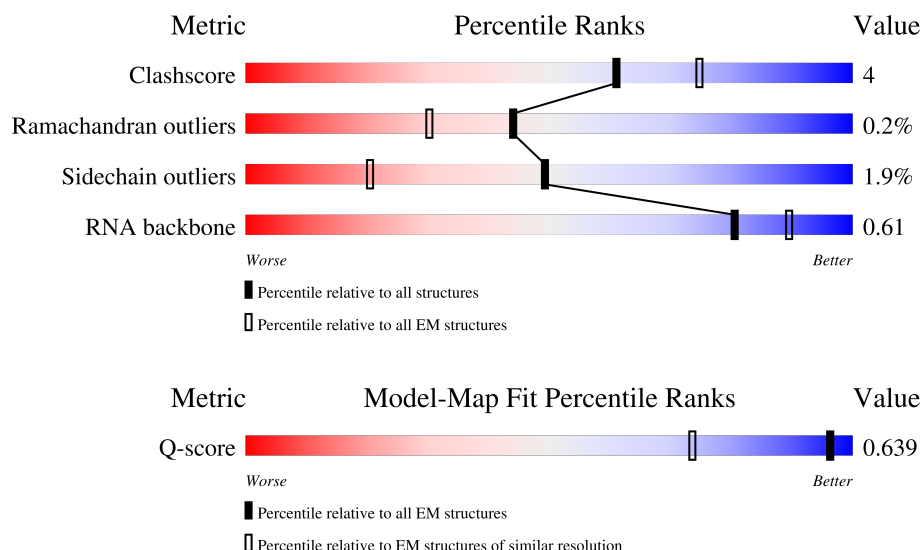
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

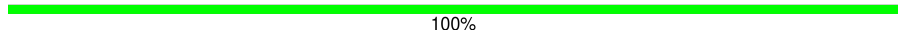
The reported resolution of this entry is 2.21 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	3231 (1.71 - 2.71)

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	0	51	 90% 8%
2	1	44	 100%
3	2	64	 94% 5%

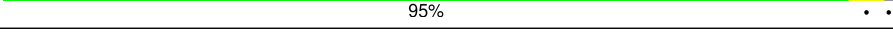
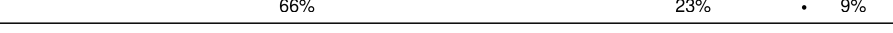
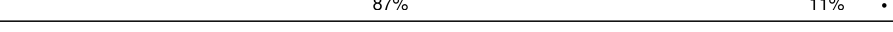
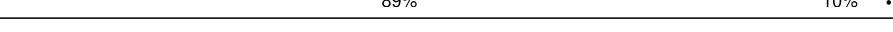
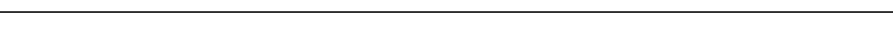
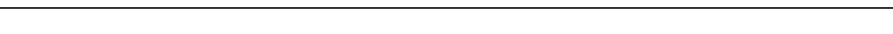
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Mol	Chain	Length	Quality of chain
4	3	38	100%
5	A	2918	68% 23% 7%
6	B	115	71% 22% 7%
7	C	274	93% 5%
8	D	212	94% 6%
9	E	200	92% 7%
10	F	178	61% 34% ..
11	G	177	78% 20% .
12	H	148	7% 37% 59%
13	I	142	94% 6%
14	J	122	94% 6%
15	K	146	92% 6%
16	L	137	94% 6%
17	M	125	93% 5%
18	N	116	85% 13% ..
19	O	122	84% 11% . .
20	P	119	94% . .
21	Q	103	88% 12%
22	R	109	93% 7%
23	S	106	78% 8% 14%
24	T	105	89% 9% ..
25	U	98	89% 10% .
26	V	85	81% 8% 11%
27	W	78	87% 13%
28	X	65	75% 14% 8%

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Mol	Chain	Length	Quality of chain
29	Y	58	
30	Z	61	
31	a	1544	
32	b	250	
33	c	250	
34	d	208	
35	e	165	
36	f	127	
37	g	156	
38	h	131	
39	i	128	
40	j	103	
41	k	128	
42	l	124	
43	m	118	
44	n	101	
45	o	89	
46	p	101	
47	q	85	
48	r	75	
49	s	91	
50	t	88	
51	u	71	

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 137191 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 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	51	Total	C	N	O	S	0	0
			427	274	77	73	3		

- Molecule 2 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	44	Total	C	N	O	S	0	0
			363	222	85	54	2		

- Molecule 3 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	63	Total	C	N	O	S	0	0
			509	319	110	76	4		

- Molecule 4 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	38	Total	C	N	O	S	0	0
			295	179	64	48	4		

- Molecule 5 is a RNA chain called 23s ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	2726	Total	C	N	O	P	0	0
			58481	26105	10707	18943	2726		

- Molecule 6 is a RNA chain called 5s ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	115	Total	C	N	O	P	0	0
			2450	1095	440	800	115		

- Molecule 7 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	271	Total	C	N	O	S	0	0
			2106	1297	436	365	8		

- Molecule 8 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	211	Total	C	N	O	S	0	0
			1572	972	297	300	3		

- Molecule 9 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	200	Total	C	N	O	S	0	0
			1516	952	281	278	5		

- Molecule 10 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	174	Total	C	N	O	S	0	0
			1370	871	243	248	8		

- Molecule 11 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	174	Total	C	N	O	S	0	0
			1318	832	236	249	1		

- Molecule 12 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	60	Total	C	N	O	S	0	0
			458	287	84	86	1		

- Molecule 13 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	142	Total	C	N	O	S	0	0
			1125	718	200	203	4		

- Molecule 14 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	122	Total	C	N	O	S	0	0
			946	592	180	169	5		

- Molecule 15 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	144	Total	C	N	O		0	0
			1071	663	213	195			

- Molecule 16 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	137	Total	C	N	O	S	0	0
			1087	687	210	185	5		

- Molecule 17 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	119	Total	C	N	O	S	0	0
			942	590	186	163	3		

- Molecule 18 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	115	Total	C	N	O	S	0	0
			865	532	175	157	1		

- Molecule 19 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	117	Total	C	N	O		0	0
			919	578	177	164			

- Molecule 20 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	117	Total	C	N	O	S	0	0
			934	589	197	146	2		

- Molecule 21 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	103	Total	C	N	O	S	0	0
			807	506	155	143	3		

- Molecule 22 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	109	Total	C	N	O	S	0	0
			826	514	158	150	4		

- Molecule 23 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	91	Total	C	N	O	S	0	0
			710	452	128	129	1		

- Molecule 24 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	103	Total	C	N	O	S	0	0
			766	476	142	148			

- Molecule 25 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	97	Total	C	N	O	S	0	0
			760	477	143	139	1		

- Molecule 26 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	V	76	Total	C	N	O	S	0	0
			577	358	111	106	2		

- Molecule 27 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	W	78	Total	C	N	O	S	0	0
			640	400	131	106	3		

- Molecule 28 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	60	Total	C	N	O	S	0	0
			486	302	93	90	1		

- Molecule 29 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	57	Total	C	N	O	S	0	0
			455	281	87	84	3		

- Molecule 30 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z	54	Total	C	N	O	S	0	0
			447	265	100	81	1		

- Molecule 31 is a RNA chain called 16s Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	1528	Total	C	N	O	P	0	0
			32782	14631	5994	10630	1527		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	1007	U	C	conflict	GB 1211343212
a	1034	C	U	conflict	GB 1211343212

- Molecule 32 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	b	225	Total	C	N	O	S	0	0
			1769	1110	328	325	6		

- Molecule 33 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	215	Total	C	N	O	S	0	0
			1690	1065	318	299	8		

- Molecule 34 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	d	207	Total	C	N	O	S	0	0
			1631	1017	313	299	2		

- Molecule 35 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	e	155	Total	C	N	O	S	0	0
			1129	700	217	207	5		

- Molecule 36 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	f	104	Total	C	N	O	S	0	0
			867	546	158	159	4		

- Molecule 37 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	136	Total	C	N	O	S	0	0
			1073	671	201	194	7		

- Molecule 38 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	130	Total	C	N	O	S	0	0
			985	615	177	187	6		

- Molecule 39 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	126	Total	C	N	O	S	0	0
			991	618	197	175	1		

- Molecule 40 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	100	Total	C	N	O	S	0	0
			801	500	150	148	3		

- Molecule 41 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	k	117	Total	C	N	O	S	0	0
			862	535	167	159	1		

- Molecule 42 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	l	122	Total	C	N	O	S	0	0
			945	580	193	167	5		

- Molecule 43 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	115	Total	C	N	O	S	0	0
			903	558	184	158	3		

- Molecule 44 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	n	100	Total	C	N	O	S	0	0
			792	493	158	137	4		

- Molecule 45 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	88	Total	C	N	O	S	0	0
			705	434	144	126	1		

- Molecule 46 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	p	82	Total	C	N	O	S	0	0
			644	403	128	112	1		

- Molecule 47 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	q	79	Total	C	N	O	S	0	0
			621	390	116	114	1		

- Molecule 48 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	r	52	Total	C	N	O	0	0
			426	273	74	79		

- Molecule 49 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	s	82	Total	C	N	O	S	0	0
			646	412	125	107	2		

- Molecule 50 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	t	86	Total	C	N	O	S	0	0
			663	409	139	113	2		

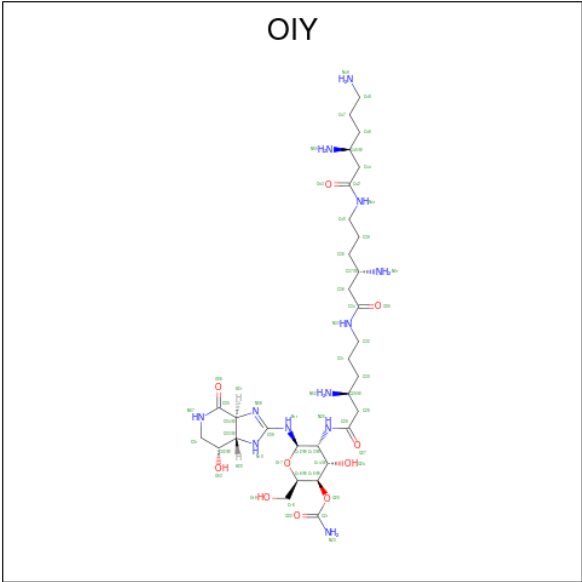
- Molecule 51 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	u	62	Total	C	N	O	S	0	0
			515	322	104	88	1		

- Molecule 52 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
52	3	1	Total	Zn	0
			1	1	

- Molecule 53 is Streptothricin D (CCD ID: OIY) (formula: C₃₁H₅₈N₁₂O₁₀) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
53	A	1	Total	C	N	O	0
			35	19	8	8	
53	A	1	Total	C	N	O	0
			35	19	8	8	
53	A	1	Total	C	N	O	0
			31	16	7	8	
53	A	1	Total	C	N	O	0
			53	31	12	10	
53	A	1	Total	C	N	O	0
			53	31	12	10	
53	A	1	Total	C	N	O	0
			40	22	9	9	
53	A	1	Total	C	N	O	0
			40	22	9	9	
53	W	1	Total	C	N	O	0
			53	31	12	10	
53	a	1	Total	C	N	O	0
			35	19	8	8	
53	a	1	Total	C	N	O	0
			53	31	12	10	
53	a	1	Total	C	N	O	0
			53	31	12	10	
53	a	1	Total	C	N	O	0
			35	19	8	8	

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
54	A	1	Total 1	Mg 1	0

- Molecule 55 is water.

Mol	Chain	Residues	Atoms		AltConf
55	A	4	Total 4	O 4	0
55	R	1	Total 1	O 1	0

3 Residue-property plots [i](#)

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

- Molecule 1: 50S ribosomal protein L33

Chain 0: 



- Molecule 2: 50S ribosomal protein L34

Chain 1: 

There are no outlier residues recorded for this chain.

- Molecule 3: 50S ribosomal protein L35

Chain 2: 



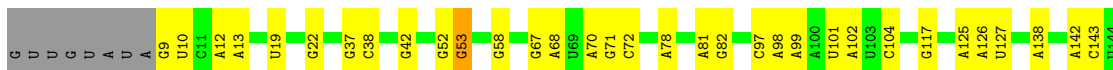
- Molecule 4: 50S ribosomal protein L36

Chain 3: 

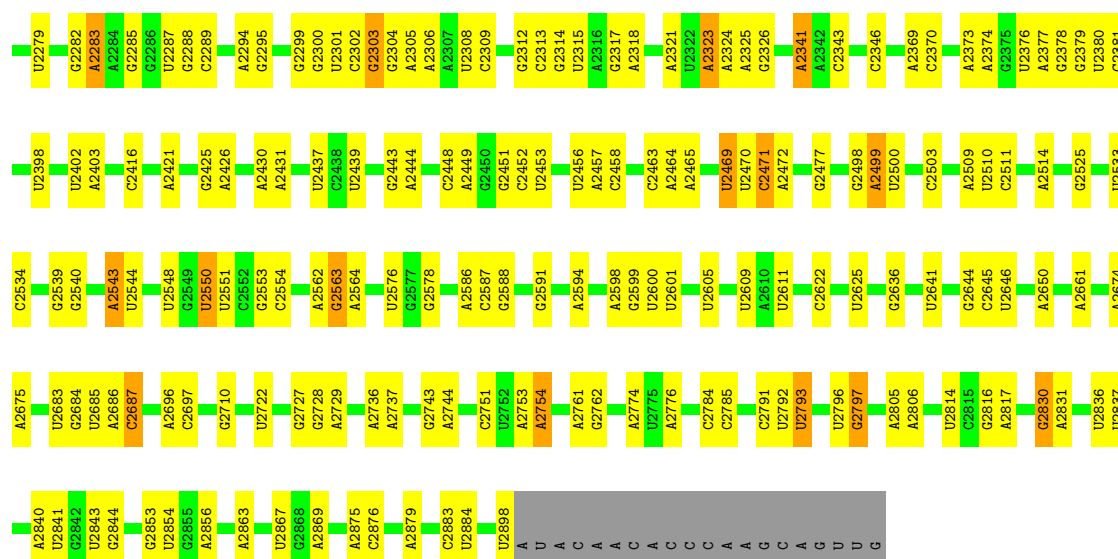
There are no outlier residues recorded for this chain.

- Molecule 5: 23s ribosomal RNA

Chain A: 

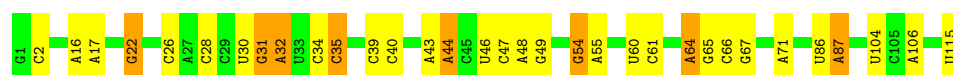






• Molecule 6: 5s ribosomal RNA

Chain B: 71% 22% 7%



• Molecule 7: 50S ribosomal protein L2

Chain C: 93% 5%



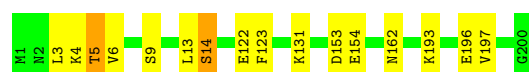
• Molecule 8: 50S ribosomal protein L3

Chain D: 94% 6%



• Molecule 9: 50S ribosomal protein L4

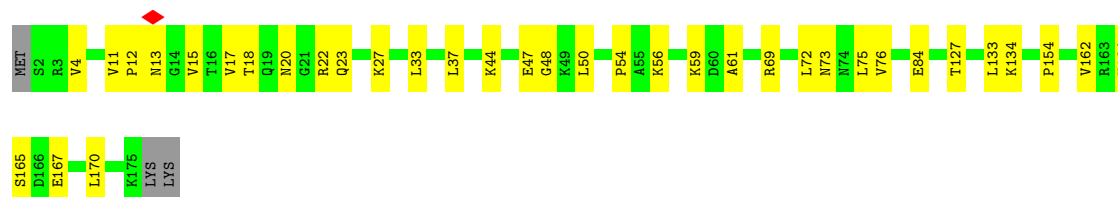
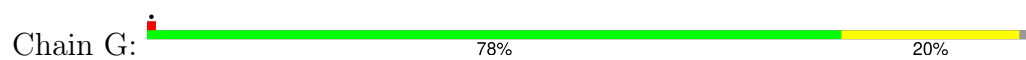
Chain E: 92% 7%



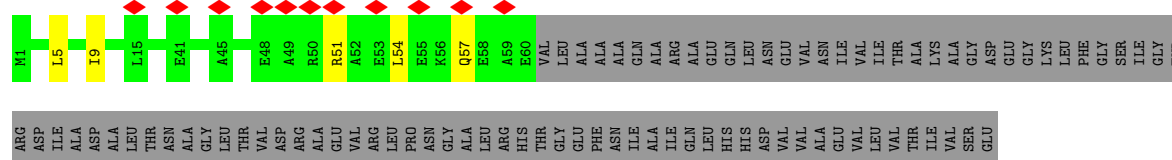
• Molecule 10: 50S ribosomal protein L5

Chain F: 61% 34% 5%

- Molecule 11: 50S ribosomal protein L6



- Molecule 12: 50S ribosomal protein L9



- Molecule 13: 50S ribosomal protein L13

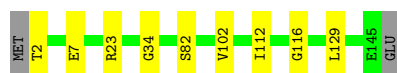


- Molecule 14: 50S ribosomal protein L14



- Molecule 15: 50S ribosomal protein L15





- Molecule 16: 50S ribosomal protein L16

Chain L: 94% 6%



- Molecule 17: 50S ribosomal protein L17

Chain M: 93% 5%



- Molecule 18: 50S ribosomal protein L18

Chain N: 85% 13% ..



- Molecule 19: 50S ribosomal protein L19

Chain O: 84% 11% . .



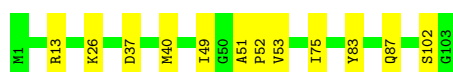
- Molecule 20: 50S ribosomal protein L20

Chain P: 94% . .



- Molecule 21: 50S ribosomal protein L21

Chain Q: 88% 12%

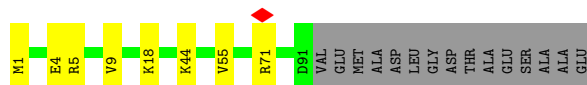
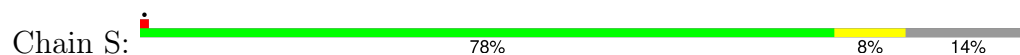


- Molecule 22: 50S ribosomal protein L22

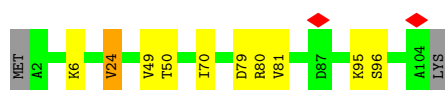
Chain R: 93% 7%



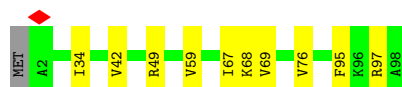
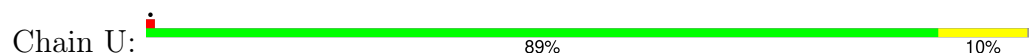
- Molecule 23: 50S ribosomal protein L23



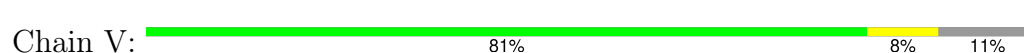
- Molecule 24: 50S ribosomal protein L24



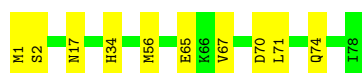
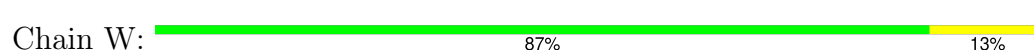
- Molecule 25: 50S ribosomal protein L25



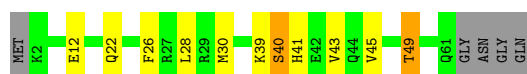
- Molecule 26: 50S ribosomal protein L27



- Molecule 27: 50S ribosomal protein L28

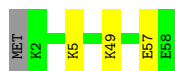


- Molecule 28: 50S ribosomal protein L29



- Molecule 29: 50S ribosomal protein L30





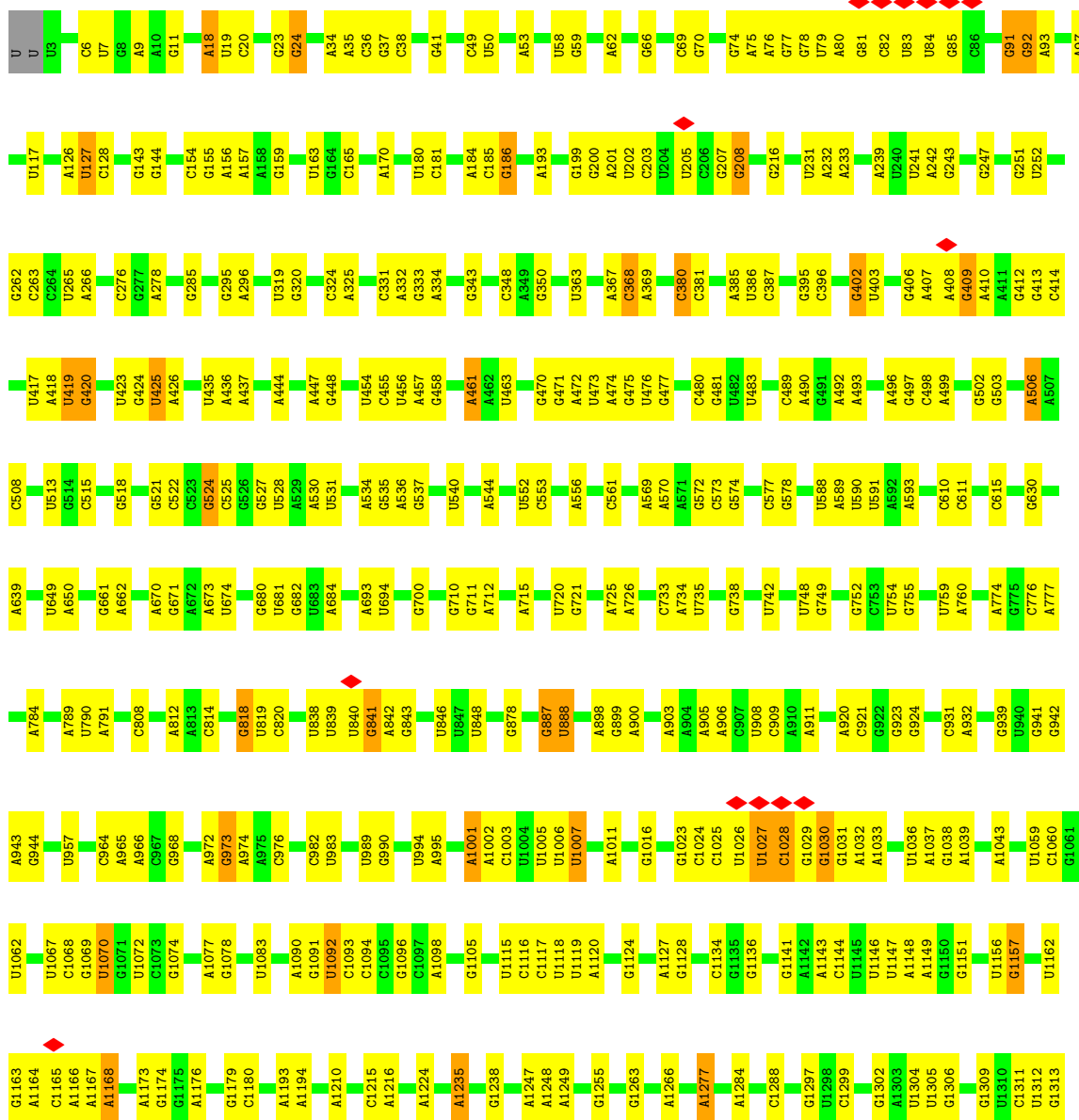
- Molecule 30: 50S ribosomal protein L32

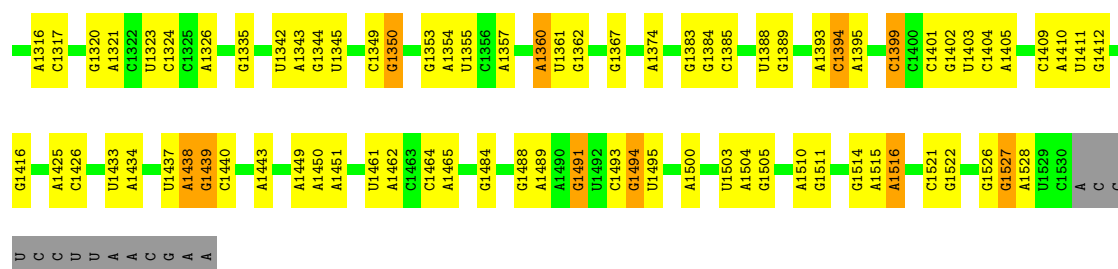
Chain Z: 79% 10% 11%



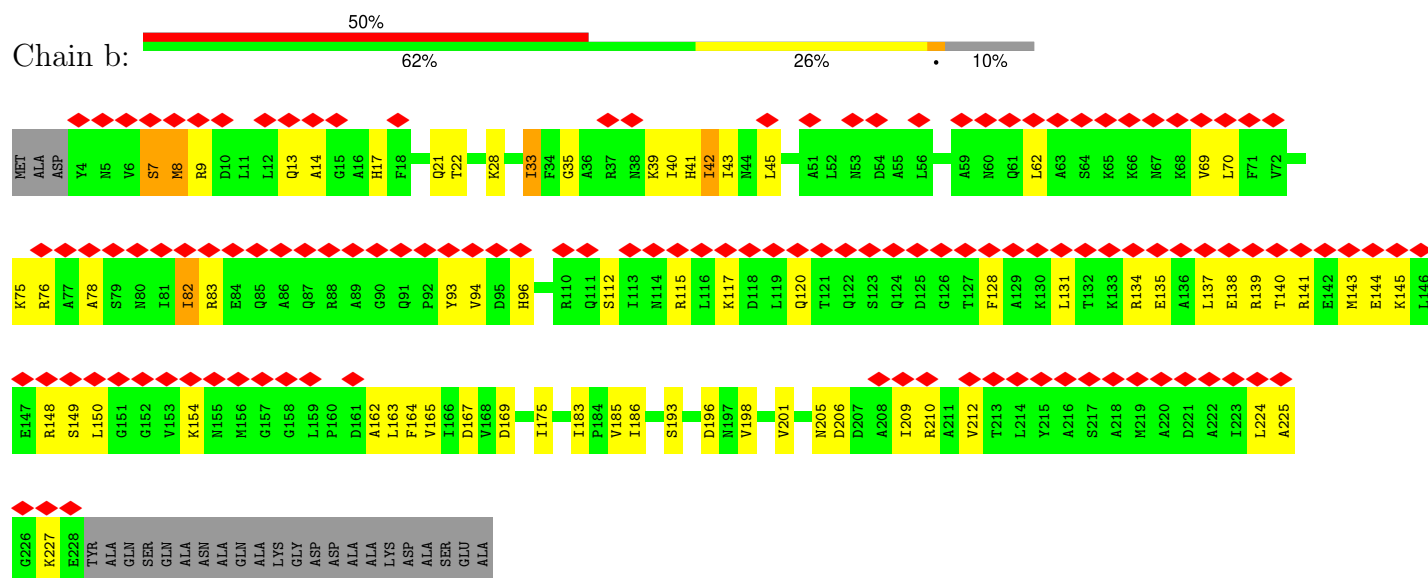
- Molecule 31: 16s Ribosomal RNA

Chain a: 68% 28% 4%

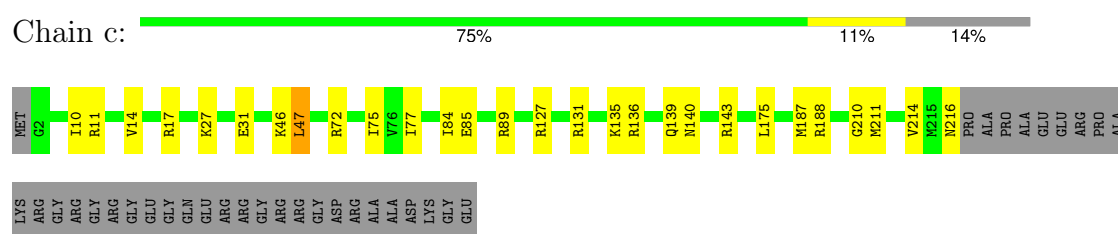




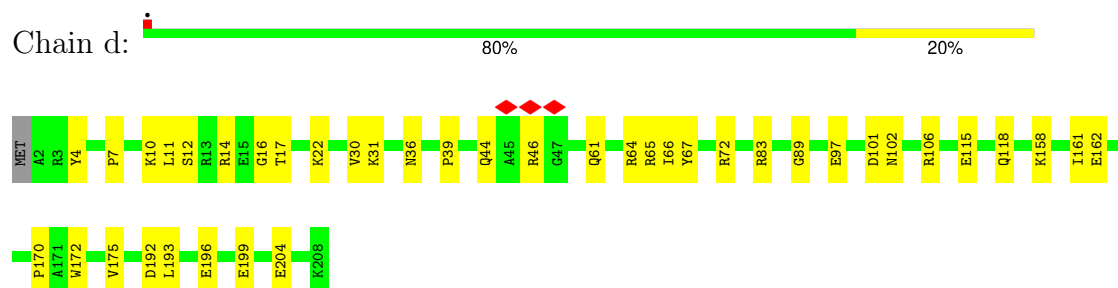
• Molecule 32: 30S ribosomal protein S2



• Molecule 33: 30S ribosomal protein S3



• Molecule 34: 30S ribosomal protein S4



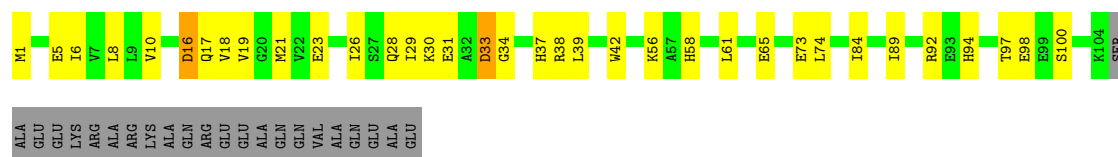
• Molecule 35: 30S ribosomal protein S5

Chain e: 



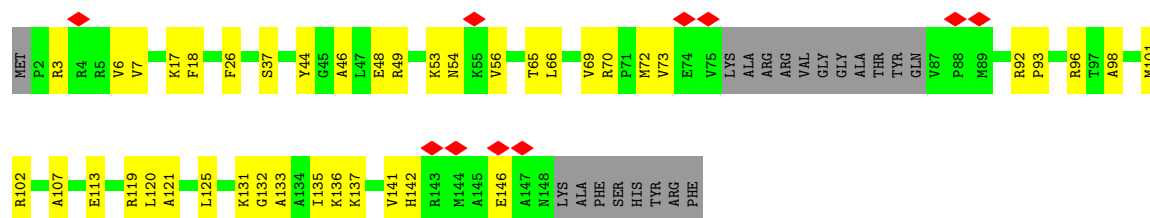
- Molecule 36: 30S ribosomal protein S6

Chain f: 

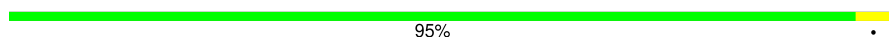


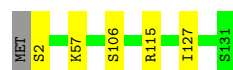
- Molecule 37: 30S ribosomal protein S7

Chain g: 



- Molecule 38: 30S ribosomal protein S8

Chain h: 



- Molecule 39: 30S ribosomal protein S9

Chain i: 



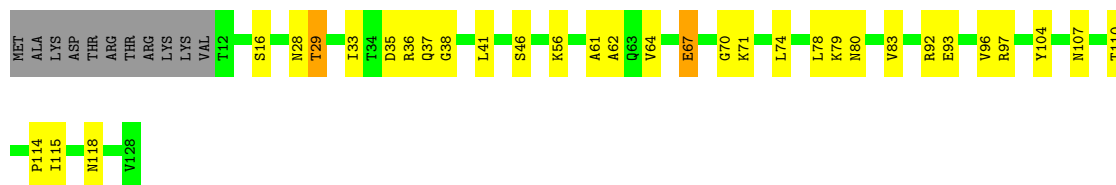
- Molecule 40: 30S ribosomal protein S10

Chain j: 



- Molecule 41: 30S ribosomal protein S11

Chain k:  66% 23% 9%



- Molecule 42: 30S ribosomal protein S12

Chain l:  87% 11%



- Molecule 43: 30S ribosomal protein S13

Chain m:  86% 11%



- Molecule 44: 30S ribosomal protein S14

Chain n:  89% 10%



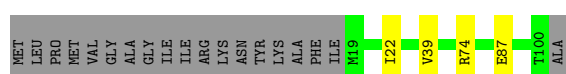
- Molecule 45: 30S ribosomal protein S15

Chain o:  85% 13%



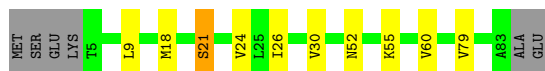
- Molecule 46: 30S ribosomal protein S16

Chain p:  77% 19%



- Molecule 47: 30S ribosomal protein S17

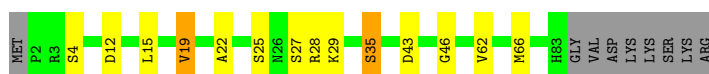
Chain q:  81% 11% 7%



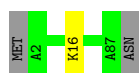
- Molecule 48: 30S ribosomal protein S18



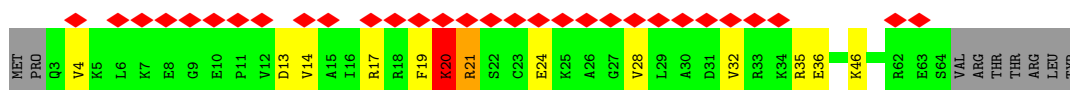
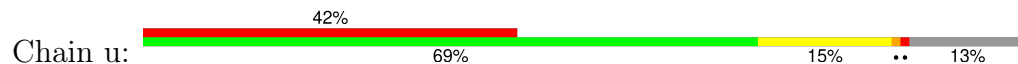
- Molecule 49: 30S ribosomal protein S19



- Molecule 50: 30S ribosomal protein S20



- Molecule 51: 30S ribosomal protein S21



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	420107	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	36	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.921	Depositor
Minimum map value	-0.027	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.08	Depositor
Map size ($\text{\AA}$)	460.80002, 460.80002, 460.80002	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.72, 0.72, 0.72	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3TD, 7MG, 6MZ, 5MU, 2MA, ZN, MG, UR3, OIY, MA6, 4OC, PSU, OMU, 5MC, OMG, 2MG

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	0	0.15	0/434	0.34	0/573
2	1	0.14	0/367	0.33	0/481
3	2	0.15	0/515	0.35	0/678
4	3	0.15	0/296	0.31	0/389
5	A	0.19	0/65134	0.30	0/101588
6	B	0.15	0/2739	0.29	0/4266
7	C	0.17	0/2146	0.38	0/2880
8	D	0.17	0/1590	0.36	0/2142
9	E	0.16	0/1537	0.34	0/2073
10	F	0.17	0/1390	0.47	0/1863
11	G	0.17	0/1337	0.41	0/1807
12	H	0.19	0/461	0.56	0/616
13	I	0.17	0/1151	0.36	0/1551
14	J	0.17	0/956	0.32	0/1286
15	K	0.16	0/1079	0.34	0/1439
16	L	0.15	0/1104	0.34	0/1475
17	M	0.17	0/956	0.38	0/1282
18	N	0.16	0/873	0.38	0/1167
19	O	0.16	0/931	0.33	0/1249
20	P	0.18	0/947	0.34	0/1262
21	Q	0.16	0/818	0.35	0/1094
22	R	0.15	0/831	0.32	0/1113
23	S	0.15	0/716	0.30	0/957
24	T	0.15	0/770	0.34	0/1034
25	U	0.15	0/770	0.35	0/1036
26	V	0.17	0/585	0.33	0/783
27	W	0.16	0/650	0.39	0/866
28	X	0.15	0/487	0.33	0/646
29	Y	0.15	0/460	0.27	0/614
30	Z	0.15	0/453	0.34	0/604
31	a	0.17	0/36476	0.27	0/56895
32	b	0.19	0/1799	0.53	0/2429

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	c	0.16	0/1714	0.37	0/2304
34	d	0.15	0/1653	0.36	0/2213
35	e	0.16	0/1141	0.38	0/1537
36	f	0.16	0/882	0.42	0/1189
37	g	0.19	0/1087	0.50	0/1456
38	h	0.16	0/993	0.30	0/1331
39	i	0.16	0/1002	0.35	0/1339
40	j	0.17	0/811	0.41	0/1096
41	k	0.19	0/878	0.47	0/1189
42	l	0.17	0/958	0.42	0/1284
43	m	0.15	0/913	0.43	0/1226
44	n	0.17	0/803	0.34	0/1071
45	o	0.16	0/715	0.31	0/958
46	p	0.17	0/655	0.37	0/879
47	q	0.16	0/628	0.40	0/847
48	r	0.16	0/432	0.39	0/583
49	s	0.17	0/664	0.33	0/897
50	t	0.19	0/669	0.27	0/892
51	u	0.22	0/520	0.70	4/686 (0.6%)
All	All	0.18	0/147876	0.32	4/221115 (0.0%)

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
21	Q	0	1
51	u	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	u	20	LYS	CA-C-N	-6.86	111.22	122.54
51	u	20	LYS	C-N-CA	-6.86	111.22	122.54
51	u	21	ARG	CB-CG-CD	6.62	126.53	111.30
51	u	21	ARG	N-CA-CB	5.84	119.13	110.49

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	Q	51	ALA	Peptide
51	u	20	LYS	Peptide

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	0	427	0	462	4	0
2	1	363	0	401	0	0
3	2	509	0	566	2	0
4	3	295	0	326	0	0
5	A	58481	0	29410	329	0
6	B	2450	0	1241	15	0
7	C	2106	0	2170	11	0
8	D	1572	0	1610	7	0
9	E	1516	0	1569	9	0
10	F	1370	0	1420	46	0
11	G	1318	0	1373	19	0
12	H	458	0	480	5	0
13	I	1125	0	1148	4	0
14	J	946	0	1007	4	0
15	K	1071	0	1141	5	0
16	L	1087	0	1162	3	0
17	M	942	0	987	2	0
18	N	865	0	905	9	0
19	O	919	0	973	12	0
20	P	934	0	997	4	0
21	Q	807	0	842	6	0
22	R	826	0	894	3	0
23	S	710	0	768	6	0
24	T	766	0	816	5	0
25	U	760	0	783	7	0
26	V	577	0	580	3	0
27	W	640	0	679	7	0
28	X	486	0	528	7	0
29	Y	455	0	476	1	0
30	Z	447	0	435	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	a	32782	0	16508	238	0
32	b	1769	0	1787	48	0
33	c	1690	0	1774	20	0
34	d	1631	0	1691	31	0
35	e	1129	0	1174	11	0
36	f	867	0	868	23	0
37	g	1073	0	1118	27	0
38	h	985	0	1047	3	0
39	i	991	0	1048	10	0
40	j	801	0	832	8	0
41	k	862	0	877	22	0
42	l	945	0	998	8	0
43	m	903	0	962	8	0
44	n	792	0	833	7	0
45	o	705	0	712	8	0
46	p	644	0	655	3	0
47	q	621	0	665	4	0
48	r	426	0	447	7	0
49	s	646	0	663	10	0
50	t	663	0	715	1	0
51	u	515	0	557	13	0
52	3	1	0	0	0	0
53	A	287	0	0	4	0
53	W	53	0	0	1	0
53	a	176	0	0	3	0
54	A	1	0	0	0	0
55	A	4	0	0	0	0
55	R	1	0	0	0	0
All	All	137191	0	92080	989	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 4.

All (989) 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)
31:a:75:A:N6	31:a:92:G:H1	1.57	1.03
31:a:1007:U:H3	31:a:1016:G:H1	1.05	0.96
5:A:2840:A:HO2'	19:O:2:SER:N	1.63	0.95
31:a:74:G:H1	31:a:93:A:H61	1.10	0.91
5:A:2300:G:H22	5:A:2308:U:H3	1.18	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2095:U:H3	5:A:2186:G:H1	1.19	0.86
31:a:333:G:N7	53:a:1601:OIY:N52	2.27	0.83
37:g:70:ARG:HG2	37:g:96:ARG:HB3	1.61	0.82
5:A:1036:A:H61	5:A:1113:G:H1	1.28	0.80
37:g:93:PRO:HA	37:g:96:ARG:HD2	1.62	0.80
18:N:59:LEU:HD21	18:N:72:LYS:HD3	1.64	0.80
37:g:132:GLY:H	37:g:136:LYS:NZ	1.80	0.80
31:a:74:G:H1	31:a:93:A:N6	1.82	0.77
31:a:75:A:H61	31:a:92:G:H1	0.81	0.77
41:k:16:SER:HB3	41:k:79:LYS:HE3	1.68	0.75
5:A:2093:U:H3	5:A:2188:G:H1	0.79	0.74
33:c:72:ARG:HB3	33:c:75:ILE:HD13	1.70	0.74
5:A:2294:A:H61	5:A:2314:G:H1	1.36	0.73
31:a:1162:U:H3	31:a:1168:A:H61	1.36	0.73
11:G:44:LYS:HE3	11:G:44:LYS:HA	1.72	0.71
32:b:120:GLN:HA	32:b:143:MET:HE1	1.70	0.71
31:a:409:G:N2	31:a:425:U:OP2	2.20	0.71
12:H:51:ARG:HA	12:H:51:ARG:HE	1.56	0.71
9:E:3:LEU:HD12	9:E:13:LEU:HD12	1.73	0.70
31:a:489:C:H2'	31:a:490:A:C8	2.26	0.70
10:F:8:TYR:HA	10:F:12:LEU:HD23	1.72	0.70
31:a:402:G:H21	34:d:118:GLN:HE22	1.40	0.69
37:g:53:LYS:HE3	37:g:54:ASN:HD22	1.58	0.69
5:A:2287:U:H2'	5:A:2288:G:C8	2.28	0.69
7:C:272:ARG:HA	7:C:272:ARG:HH11	1.57	0.69
36:f:92:ARG:HG2	36:f:92:ARG:HH11	1.59	0.68
24:T:49:VAL:HG23	24:T:50:THR:HG23	1.75	0.68
31:a:841:G:H1'	31:a:842:A:C8	2.28	0.68
5:A:1108:A:H8	5:A:1109:G:H1'	1.58	0.68
37:g:132:GLY:H	37:g:136:LYS:HZ1	1.40	0.68
7:C:135:MET:O	7:C:167:ARG:NH2	2.25	0.68
32:b:9:ARG:HH12	32:b:13:GLN:HG2	1.59	0.68
34:d:11:LEU:HG	34:d:65:ARG:HE	1.58	0.68
10:F:15:LYS:NZ	10:F:19:GLU:OE1	2.27	0.68
5:A:1908:A:O2'	31:a:1491:G:O2'	2.12	0.67
20:P:43:GLY:HA3	21:Q:75:ILE:HD12	1.76	0.67
9:E:122:GLU:OE2	9:E:123:PHE:N	2.28	0.67
5:A:2644:G:N7	53:A:3002:OIY:N52	2.42	0.67
28:X:45:VAL:O	28:X:49:THR:OG1	2.13	0.67
31:a:710:G:H2'	31:a:711:G:C8	2.30	0.67
31:a:1311:C:OP2	49:s:4:SER:OG	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:471:G:H2'	31:a:472:A:C8	2.30	0.67
7:C:271:ARG:O	7:C:272:ARG:HB2	1.96	0.66
32:b:7:SER:OG	32:b:8:MET:N	2.29	0.66
10:F:110:ARG:HD2	10:F:137:VAL:HA	1.75	0.66
10:F:56:ASP:O	10:F:60:ILE:HD12	1.96	0.66
5:A:2093:U:O2	5:A:2188:G:N2	2.20	0.65
42:l:123:LYS:H	42:l:123:LYS:HE2	1.61	0.65
33:c:136:ARG:HG3	33:c:136:ARG:HH11	1.61	0.65
36:f:26:ILE:HD11	36:f:39:LEU:HD13	1.79	0.65
33:c:75:ILE:HD12	33:c:75:ILE:H	1.61	0.65
43:m:3:ARG:NH1	43:m:8:ASN:OD1	2.30	0.65
5:A:1044:G:O2'	5:A:1108:A:N6	2.28	0.65
30:Z:52:GLN:HE22	30:Z:54:PHE:C	2.05	0.65
5:A:322:G:N7	9:E:131:LYS:NZ	2.44	0.65
29:Y:5:LYS:NZ	29:Y:57:GLU:OE1	2.30	0.65
10:F:122:PHE:HE2	10:F:167:ARG:HG3	1.62	0.64
5:A:1854:A:H61	5:A:1880:G:H1'	1.61	0.64
31:a:943:A:H2'	31:a:944:G:C8	2.32	0.64
5:A:1595:A:H5''	5:A:1596:A:H5'	1.79	0.64
10:F:162:THR:OG1	10:F:163:ASP:N	2.29	0.64
31:a:207:G:O2'	31:a:208:G:O4'	2.14	0.64
5:A:854:G:H2'	5:A:855:G:C8	2.33	0.64
5:A:2309:C:O4'	10:F:37:ASN:ND2	2.31	0.64
31:a:1527:G:N7	51:u:46:LYS:NZ	2.45	0.64
5:A:1726:C:H4'	5:A:1727:G:H5'	1.79	0.64
27:W:17:ASN:OD1	53:W:101:OIY:N49	2.31	0.64
40:j:10:LEU:HD22	40:j:98:VAL:HG22	1.79	0.64
41:k:92:ARG:HH21	51:u:20:LYS:HD3	1.61	0.64
5:A:2063:G:H1	5:A:2439:U:H3	1.47	0.63
5:A:1036:A:N6	5:A:1113:G:H1	1.97	0.63
33:c:85:GLU:OE1	33:c:89:ARG:NH1	2.32	0.63
5:A:284:U:H3	5:A:360:A:H62	1.47	0.63
12:H:5:LEU:HD22	12:H:9:ILE:HD13	1.79	0.63
30:Z:52:GLN:NE2	30:Z:54:PHE:O	2.31	0.63
11:G:164:TYR:HB2	11:G:167:GLU:HB2	1.81	0.63
31:a:994:U:H2'	31:a:995:A:H8	1.64	0.63
10:F:56:ASP:OD2	10:F:150:ARG:NH1	2.32	0.62
5:A:2048:A:H4'	8:D:151:GLN:O	1.99	0.62
5:A:2465:A:N6	5:A:2477:G:O2'	2.32	0.62
31:a:423:U:OP2	31:a:424:G:O2'	2.14	0.62
31:a:733:C:H2'	31:a:734:A:H8	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2324:A:H2'	5:A:2325:A:C8	2.35	0.62
31:a:1163:G:O2'	31:a:1167:A:N6	2.33	0.62
35:e:110:MET:HE2	35:e:126:CYS:SG	2.40	0.62
10:F:141:ILE:HG21	10:F:145:LYS:HE3	1.80	0.62
31:a:1083:U:H3	31:a:1096:G:H22	1.46	0.62
51:u:17:ARG:HB3	51:u:21:ARG:HH12	1.63	0.62
33:c:140:ASN:OD1	33:c:143:ARG:NH2	2.32	0.61
20:P:97:ASP:OD2	21:Q:13:ARG:NH1	2.32	0.61
5:A:368:C:H4'	5:A:369:G:O5'	2.00	0.61
31:a:661:G:H22	31:a:738:G:H1	1.46	0.61
5:A:1185:G:H5'	15:K:34:GLY:HA2	1.81	0.61
33:c:211:MET:SD	33:c:216:ASN:ND2	2.73	0.61
31:a:820:C:HO2'	38:h:2:SER:N	1.99	0.61
5:A:1044:G:H21	5:A:1108:A:H2	1.49	0.61
41:k:46:SER:HB3	41:k:61:ALA:HB1	1.83	0.61
5:A:579:C:H2'	5:A:580:A:H8	1.66	0.60
32:b:69:VAL:HG22	32:b:162:ALA:HB3	1.82	0.60
34:d:162:GLU:O	34:d:166:GLN:NE2	2.34	0.60
41:k:29:THR:HG21	41:k:62:ALA:HB2	1.84	0.60
33:c:77:ILE:HD13	33:c:84:ILE:HG21	1.83	0.60
5:A:579:C:H2'	5:A:580:A:C8	2.37	0.60
53:A:3005:OIY:N50	53:A:3005:OIY:O43	2.34	0.60
5:A:1428:A:H2'	5:A:1429:A:C8	2.37	0.59
39:i:37:PHE:O	39:i:43:ARG:NH1	2.35	0.59
49:s:22:ALA:O	49:s:25:SER:O	2.20	0.59
5:A:2308:U:O2	10:F:37:ASN:ND2	2.35	0.59
10:F:12:LEU:HD12	10:F:172:ALA:HB1	1.82	0.59
31:a:1461:U:H2'	31:a:1462:A:H8	1.67	0.59
31:a:1263:G:N2	31:a:1266:A:OP2	2.33	0.59
37:g:142:HIS:O	37:g:146:GLU:HG2	2.01	0.59
12:H:51:ARG:HA	12:H:51:ARG:NE	2.15	0.59
31:a:1036:U:H2'	31:a:1037:A:H8	1.68	0.59
42:l:65:SER:HG	42:l:97:THR:HG1	1.49	0.59
5:A:714:A:OP1	45:o:88:ARG:NH2	2.33	0.59
31:a:711:G:H2'	31:a:712:A:C8	2.38	0.59
43:m:37:VAL:HG23	43:m:39:ILE:HG13	1.85	0.59
5:A:1464:A:H2'	5:A:1465:A:C8	2.38	0.59
13:I:114:LEU:HG	13:I:118:MET:HE3	1.85	0.59
31:a:143:G:H2'	31:a:144:G:C8	2.38	0.59
49:s:12:ASP:OD2	49:s:35:SER:OG	2.21	0.59
5:A:2543:A:H2'	5:A:2544:U:C6	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:c:84:ILE:HD12	33:c:85:GLU:N	2.18	0.58
5:A:2294:A:N1	5:A:2314:G:N2	2.50	0.58
31:a:498:C:H2'	31:a:499:A:H8	1.68	0.58
31:a:733:C:H2'	31:a:734:A:C8	2.39	0.58
11:G:54:PRO:HB3	11:G:61:ALA:HB1	1.85	0.58
6:B:26:C:H5''	18:N:32:THR:HG21	1.85	0.58
32:b:117:LYS:HE3	32:b:154:LYS:HB2	1.85	0.58
32:b:131:LEU:HD12	32:b:135:GLU:HB3	1.86	0.58
49:s:28:ARG:NH1	49:s:46:GLY:O	2.37	0.58
5:A:2325:A:H2'	5:A:2326:G:C8	2.39	0.58
5:A:2469:U:OP1	5:A:2471:C:N4	2.36	0.58
31:a:649:U:O4	31:a:749:G:O2'	2.22	0.57
49:s:15:LEU:O	49:s:19:VAL:HG13	2.04	0.57
31:a:417:U:O4	33:c:127:ARG:NH2	2.37	0.57
31:a:670:A:H2'	31:a:671:G:C8	2.39	0.57
31:a:1320:G:H2'	31:a:1321:A:C8	2.40	0.57
10:F:38:MET:HE1	10:F:53:ALA:HB1	1.85	0.57
28:X:39:LYS:HB3	28:X:41:HIS:CD2	2.40	0.57
32:b:134:ARG:O	32:b:137:LEU:HG	2.04	0.57
32:b:137:LEU:HD12	32:b:141:ARG:HH21	1.70	0.57
37:g:49:ARG:HH22	37:g:125:LEU:HD11	1.68	0.57
36:f:5:GLU:OE2	48:r:24:LYS:NZ	2.37	0.57
5:A:2687:C:HO2'	5:A:2867:U:HO2'	1.49	0.57
5:A:455:C:H2'	23:S:71:ARG:HH12	1.70	0.56
32:b:140:THR:O	32:b:143:MET:HB2	2.05	0.56
5:A:1481:U:H3	5:A:1498:G:H1	1.52	0.56
5:A:52:G:H5''	5:A:53:G:H5'	1.87	0.56
5:A:1749:G:N2	5:A:1752:G:OP2	2.35	0.56
5:A:2060:C:H2'	5:A:2061:C:C6	2.40	0.56
31:a:1313:G:H4'	44:n:58:VAL:HG11	1.87	0.56
32:b:144:GLU:O	32:b:148:ARG:HG2	2.04	0.56
5:A:1037:A:H61	5:A:1112:G:H1	1.54	0.56
5:A:2587:C:H2'	5:A:2588:G:H8	1.71	0.56
49:s:22:ALA:O	49:s:25:SER:C	2.49	0.56
43:m:86:TYR:O	43:m:90:ARG:HG2	2.05	0.56
5:A:2067:A:H2'	5:A:2068:C:C6	2.41	0.56
37:g:26:PHE:HD1	37:g:101:MET:HG2	1.69	0.56
5:A:2313:C:H2'	5:A:2314:G:C8	2.41	0.56
1:0:5:ILE:HD12	1:0:47:GLU:HG3	1.88	0.56
10:F:136:ILE:O	10:F:137:VAL:HG22	2.06	0.56
35:e:114:LEU:HD13	35:e:122:VAL:HG11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:14:SER:N	9:E:196:GLU:OE2	2.38	0.55
10:F:38:MET:HG2	10:F:151:GLY:O	2.06	0.55
15:K:82:SER:HB3	15:K:116:GLY:HA3	1.87	0.55
31:a:265:U:H2'	31:a:266:A:C8	2.41	0.55
37:g:65:THR:O	37:g:69:VAL:HG23	2.06	0.55
7:C:121:ASP:OD1	7:C:121:ASP:N	2.33	0.55
36:f:16:ASP:OD1	36:f:16:ASP:N	2.31	0.55
5:A:363:G:OP2	5:A:364:A:O2'	2.21	0.55
27:W:67:VAL:O	27:W:71:LEU:HG	2.07	0.55
32:b:33:ILE:O	32:b:35:GLY:N	2.40	0.55
9:E:4:LYS:HE2	9:E:4:LYS:HA	1.88	0.55
31:a:19:U:H2'	31:a:20:C:C6	2.41	0.55
31:a:75:A:N1	31:a:92:G:N2	2.45	0.55
32:b:134:ARG:H	32:b:134:ARG:HD2	1.71	0.55
5:A:591:U:H2'	5:A:592:U:C6	2.42	0.55
5:A:578:U:H2'	5:A:579:C:C6	2.42	0.55
11:G:22:ARG:HH21	11:G:37:LEU:HD23	1.71	0.55
5:A:2315:U:O2'	5:A:2317:G:N7	2.37	0.54
41:k:93:GLU:OE2	51:u:20:LYS:NZ	2.33	0.54
10:F:112:ARG:HH21	43:m:71:ARG:HD2	1.73	0.54
5:A:741:U:O2'	5:A:1657:U:OP1	2.23	0.54
10:F:80:ARG:HB2	10:F:83:TRP:CD1	2.42	0.54
33:c:17:ARG:NH1	33:c:216:ASN:O	2.40	0.54
8:D:6:VAL:HG11	8:D:79:LEU:HD11	1.88	0.54
5:A:1041:A:O2'	5:A:1108:A:N6	2.36	0.54
10:F:166:GLY:O	10:F:170:MET:HG2	2.07	0.54
31:a:473:U:H2'	31:a:474:A:H8	1.73	0.54
5:A:831:A:H2'	5:A:832:G:C8	2.43	0.54
31:a:905:A:H2'	31:a:906:A:H8	1.73	0.54
31:a:1353:G:H2'	31:a:1354:A:C8	2.43	0.54
40:j:7:ARG:HD3	40:j:73:LEU:HD11	1.89	0.54
5:A:740:G:H2'	5:A:741:U:C6	2.43	0.54
31:a:1001:A:H2'	31:a:1002:A:O4'	2.07	0.54
5:A:2082:U:H2'	5:A:2083:G:C8	2.42	0.54
31:a:498:C:H2'	31:a:499:A:C8	2.42	0.54
5:A:413:C:H2'	5:A:414:A:C8	2.43	0.53
5:A:1849:A:H2'	5:A:1850:A:C8	2.43	0.53
5:A:2587:C:H2'	5:A:2588:G:C8	2.43	0.53
36:f:17:GLN:O	36:f:21:MET:HG3	2.07	0.53
38:h:106:SER:HB2	38:h:127:ILE:HD11	1.89	0.53
47:q:18:MET:HE3	47:q:21:SER:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:s:62:VAL:HA	49:s:66:MET:HE2	1.90	0.53
5:A:418:U:H2'	5:A:419:C:C6	2.42	0.53
5:A:413:C:H2'	5:A:414:A:H8	1.74	0.53
36:f:92:ARG:HG2	36:f:92:ARG:NH1	2.23	0.53
5:A:71:G:H2'	5:A:72:C:H6	1.72	0.53
34:d:204:GLU:OE1	35:e:111:ARG:NH1	2.41	0.53
51:u:21:ARG:HA	51:u:24:GLU:HB2	1.90	0.53
31:a:476:U:H2'	31:a:477:G:C8	2.44	0.53
5:A:2591:G:N2	5:A:2594:A:OP2	2.34	0.53
34:d:97:GLU:OE1	34:d:106:ARG:NH1	2.42	0.53
32:b:164:PHE:HA	32:b:186:ILE:O	2.09	0.53
41:k:93:GLU:CD	51:u:20:LYS:HZ2	2.16	0.53
5:A:2674:A:H2'	5:A:2675:A:C8	2.44	0.53
12:H:51:ARG:HE	12:H:51:ARG:CA	2.21	0.53
14:J:38:ILE:HD11	14:J:111:PHE:HZ	1.73	0.53
31:a:1027:U:H3'	31:a:1028:C:H4'	1.91	0.53
5:A:308:U:H2'	5:A:309:G:O4'	2.09	0.52
31:a:973:G:OP2	31:a:1355:U:O2'	2.26	0.52
5:A:1479:U:H2'	5:A:1480:A:H8	1.74	0.52
37:g:137:LYS:O	37:g:141:VAL:HG23	2.09	0.52
41:k:97:ARG:HG3	41:k:97:ARG:HH11	1.74	0.52
5:A:2093:U:O4	5:A:2188:G:O6	2.26	0.52
27:W:65:GLU:CD	27:W:65:GLU:H	2.16	0.52
5:A:2323:A:H2'	5:A:2324:A:C8	2.44	0.52
11:G:4:VAL:O	11:G:69:ARG:HD2	2.10	0.52
25:U:34:ILE:HB	25:U:42:VAL:HG23	1.90	0.52
31:a:1215:C:H2'	31:a:1216:A:C8	2.45	0.52
34:d:101:ASP:OD1	34:d:102:ASN:N	2.42	0.52
31:a:473:U:H2'	31:a:474:A:C8	2.45	0.52
31:a:1313:G:N1	31:a:1316:A:OP2	2.40	0.52
31:a:1388:U:H2'	31:a:1389:G:C8	2.44	0.52
1:0:40:ARG:HG2	1:0:40:ARG:HH11	1.73	0.52
5:A:1108:A:C8	5:A:1109:G:H1'	2.42	0.52
43:m:71:ARG:O	43:m:75:MET:HG2	2.10	0.52
51:u:14:VAL:HG22	51:u:17:ARG:NH2	2.24	0.52
31:a:127:U:H2'	31:a:128:C:C6	2.45	0.52
31:a:231:U:H2'	31:a:232:A:H8	1.74	0.52
31:a:1437:U:H2'	31:a:1438:A:C4	2.45	0.52
5:A:71:G:H2'	5:A:72:C:C6	2.45	0.52
5:A:161:A:H2'	5:A:162:A:C8	2.45	0.52
5:A:1568:A:H2'	5:A:1569:A:C8	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2308:U:H5'	10:F:85:ILE:HD11	1.91	0.52
41:k:67:GLU:O	41:k:71:LYS:HG3	2.10	0.52
5:A:1521:G:H1	5:A:1544:G:H22	1.57	0.51
18:N:31:ARG:HG3	18:N:36:ILE:HD12	1.91	0.51
5:A:846:U:H2'	5:A:847:A:H8	1.75	0.51
5:A:1503:C:H5'	5:A:1504:U:H2'	1.91	0.51
14:J:17:ARG:HD2	14:J:47:ILE:HG23	1.92	0.51
32:b:209:ILE:HD12	32:b:210:ARG:H	1.75	0.51
5:A:12:A:H2'	5:A:13:A:C8	2.45	0.51
5:A:1634:G:H2'	5:A:1635:A:C8	2.46	0.51
31:a:200:G:H2'	31:a:201:A:H8	1.76	0.51
31:a:454:U:H3	31:a:470:G:H1	1.58	0.51
49:s:27:SER:OG	49:s:29:LYS:NZ	2.39	0.51
5:A:2533:U:H2'	5:A:2534:C:C6	2.46	0.51
34:d:7:PRO:HG2	34:d:10:LYS:HD3	1.92	0.51
47:q:60:VAL:HG12	47:q:79:VAL:HG22	1.92	0.51
5:A:1182:G:H5'	21:Q:83:TYR:CE1	2.45	0.51
6:B:87:A:H2'	6:B:87:A:N3	2.25	0.51
28:X:28:LEU:HB3	28:X:43:VAL:HG12	1.92	0.51
35:e:54:GLU:OE2	35:e:54:GLU:HA	2.10	0.51
45:o:4:THR:OG1	45:o:5:ASN:N	2.44	0.51
5:A:1111:C:H2'	5:A:1112:G:C8	2.45	0.51
5:A:1854:A:N6	5:A:1880:G:H1'	2.25	0.51
31:a:725:A:H2'	31:a:726:A:C8	2.46	0.51
31:a:1409:C:H2'	31:a:1410:A:C8	2.46	0.51
32:b:21:GLN:HA	32:b:40:ILE:HA	1.92	0.51
39:i:113:LYS:HB2	39:i:116:LEU:HD12	1.92	0.51
5:A:2282:G:H4'	5:A:2283:A:O4'	2.10	0.51
21:Q:40:MET:HE3	21:Q:49:ILE:HG12	1.92	0.51
5:A:606:A:H2'	5:A:607:A:C8	2.46	0.51
5:A:2237:A:H2'	5:A:2238:G:C8	2.46	0.51
5:A:2586:A:H2'	5:A:2587:C:H6	1.75	0.51
5:A:19:U:O2	5:A:2622:C:H4'	2.11	0.51
5:A:280:A:H2'	5:A:281:A:C8	2.46	0.51
5:A:2239:U:H2'	5:A:2240:U:C6	2.46	0.51
37:g:66:LEU:HD23	37:g:70:ARG:HH21	1.76	0.51
39:i:20:SER:OG	39:i:21:ALA:N	2.41	0.50
5:A:2287:U:H2'	5:A:2288:G:H8	1.74	0.50
10:F:130:MET:HB2	10:F:154:ILE:HB	1.92	0.50
35:e:78:THR:HB	35:e:120:HIS:HB2	1.92	0.50
5:A:578:U:H2'	5:A:579:C:H6	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1792:U:H2'	5:A:1793:C:H6	1.76	0.50
10:F:118:SER:O	10:F:128:TYR:OH	2.26	0.50
5:A:847:A:H2'	5:A:848:C:C6	2.45	0.50
31:a:1120:A:O2'	40:j:39:PRO:O	2.29	0.50
48:r:36:ASN:O	48:r:72:ASP:N	2.43	0.50
31:a:1068:C:H2'	31:a:1069:G:H8	1.77	0.50
36:f:28:GLN:O	36:f:31:GLU:HG3	2.12	0.50
5:A:1036:A:O3'	25:U:49:ARG:HD2	2.12	0.50
5:A:2736:A:H2'	5:A:2737:A:C8	2.47	0.50
18:N:19:ILE:HG21	18:N:26:ARG:HG3	1.93	0.50
31:a:1026:U:H2'	31:a:1028:C:H1'	1.94	0.50
32:b:96:HIS:ND1	32:b:148:ARG:O	2.44	0.50
35:e:71:ILE:HG12	35:e:140:PHE:CZ	2.45	0.50
45:o:75:HIS:O	45:o:79:THR:HG23	2.12	0.50
5:A:782:G:H5'	5:A:783:G:OP1	2.11	0.50
5:A:1348:A:H2'	5:A:1349:A:C8	2.46	0.50
5:A:1798:A:H2'	5:A:1799:A:C8	2.46	0.50
7:C:21:HIS:NE2	7:C:199:GLU:OE2	2.40	0.50
32:b:112:SER:HA	32:b:115:ARG:CD	2.42	0.50
5:A:1527:U:H3'	5:A:1528:G:H8	1.77	0.50
31:a:610:C:H2'	31:a:611:C:C6	2.47	0.50
44:n:31:ILE:HD11	44:n:45:MET:HA	1.94	0.50
5:A:1792:U:H2'	5:A:1793:C:C6	2.46	0.50
48:r:21:ILE:HD13	48:r:55:LEU:HD12	1.94	0.50
5:A:1827:G:OP1	53:A:3003:OIY:N11	2.45	0.49
5:A:2879:A:OP2	30:Z:49:ARG:NH1	2.40	0.49
10:F:122:PHE:CE2	10:F:167:ARG:HG3	2.44	0.49
33:c:77:ILE:HA	33:c:84:ILE:HG23	1.94	0.49
35:e:63:LEU:O	35:e:67:ARG:HG3	2.13	0.49
1:0:6:ARG:HD3	1:0:50:ILE:HA	1.94	0.49
5:A:364:A:H4'	5:A:365:U:O5'	2.12	0.49
31:a:887:G:H4'	31:a:888:U:O5'	2.11	0.49
42:l:111:ASN:O	42:l:111:ASN:ND2	2.42	0.49
5:A:830:U:H2'	5:A:831:A:C8	2.47	0.49
31:a:333:G:H2'	31:a:334:A:C8	2.47	0.49
5:A:1335:U:OP1	23:S:18:LYS:NZ	2.45	0.49
31:a:156:A:H2'	31:a:157:A:O4'	2.12	0.49
36:f:8:LEU:HD22	36:f:84:ILE:HD13	1.93	0.49
3:2:30:HIS:CD2	3:2:31:ILE:HG13	2.48	0.49
5:A:2287:U:OP1	5:A:2376:U:O2'	2.31	0.49
31:a:386:U:H2'	31:a:387:C:C6	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:b:165:VAL:HG21	32:b:175:ILE:HD11	1.94	0.49
32:b:205:ASN:OD1	32:b:206:ASP:N	2.45	0.49
5:A:2095:U:O2	5:A:2186:G:N2	2.36	0.49
19:O:36:LYS:HD2	19:O:41:GLU:HG2	1.93	0.49
32:b:135:GLU:HA	32:b:138:GLU:OE2	2.13	0.49
5:A:1363:G:N7	53:A:3006:OIY:N52	2.61	0.49
5:A:1381:A:H2'	5:A:1382:U:C6	2.47	0.49
5:A:1543:A:H3'	5:A:1544:G:C8	2.48	0.49
31:a:36:C:H2'	31:a:37:G:H8	1.78	0.49
33:c:210:GLY:O	33:c:214:VAL:HG23	2.12	0.49
5:A:42:G:H8	5:A:42:G:OP2	1.95	0.49
5:A:1790:A:H2'	5:A:1791:C:C6	2.48	0.49
5:A:1790:A:H2'	5:A:1791:C:H6	1.77	0.49
5:A:1885:A:H2'	5:A:1886:A:C8	2.48	0.49
5:A:2070:U:H2'	5:A:2071:U:C6	2.48	0.49
37:g:46:ALA:HA	37:g:121:ALA:HB2	1.95	0.49
47:q:52:ASN:O	47:q:55:LYS:NZ	2.46	0.49
5:A:1166:A:H2'	5:A:1167:U:C6	2.48	0.49
25:U:34:ILE:HG12	25:U:95:PHE:HB2	1.95	0.49
5:A:862:G:H2'	5:A:863:C:C6	2.47	0.49
5:A:1167:U:H2'	5:A:1168:A:C8	2.48	0.49
31:a:232:A:H2'	31:a:233:A:C8	2.48	0.49
31:a:674:U:H3	31:a:710:G:H22	1.61	0.49
31:a:1074:G:N2	31:a:1077:A:OP2	2.39	0.49
3:2:33:THR:OG1	5:A:2416:C:OP1	2.21	0.48
5:A:637:U:H2'	5:A:638:C:C6	2.48	0.48
5:A:811:U:H2'	5:A:812:C:H6	1.78	0.48
5:A:2187:A:H2'	5:A:2188:G:H8	1.78	0.48
5:A:944:A:H2'	5:A:945:C:C6	2.48	0.48
5:A:1193:U:H2'	5:A:1194:U:C6	2.48	0.48
31:a:942:G:C2	31:a:943:A:C8	3.00	0.48
32:b:209:ILE:HD12	32:b:210:ARG:N	2.27	0.48
5:A:1879:U:H2'	5:A:1880:G:O4'	2.12	0.48
12:H:54:LEU:HD12	12:H:57:GLN:HB3	1.95	0.48
19:O:5:HIS:O	19:O:9:GLN:HG3	2.13	0.48
31:a:242:A:C2	31:a:278:A:C5	3.01	0.48
31:a:457:A:H2'	31:a:458:G:H8	1.79	0.48
31:a:1002:A:C5	31:a:1003:C:H1'	2.49	0.48
31:a:1311:C:H2'	31:a:1312:U:C6	2.48	0.48
53:a:1601:OIY:O53	53:a:1601:OIY:N33	2.47	0.48
6:B:64:A:H61	6:B:104:U:H2'	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:5:THR:HG23	9:E:9:SER:O	2.14	0.48
24:T:70:ILE:HG21	24:T:81:VAL:HG23	1.93	0.48
31:a:58:U:H2'	31:a:59:G:C8	2.49	0.48
31:a:419:U:O2'	31:a:420:G:O5'	2.31	0.48
33:c:187:MET:HG3	33:c:188:ARG:N	2.29	0.48
5:A:605:U:C5	5:A:618:G:C5	3.01	0.48
5:A:1361:A:OP1	27:W:2:SER:OG	2.32	0.48
19:O:30:VAL:HG22	19:O:47:GLU:HG3	1.96	0.48
31:a:1527:G:H2'	31:a:1528:A:C8	2.49	0.48
53:a:1602:OIY:N50	53:a:1602:OIY:O43	2.44	0.48
41:k:92:ARG:O	41:k:96:VAL:HG22	2.13	0.48
5:A:2229:U:H2'	5:A:2230:G:C8	2.49	0.48
34:d:14:ARG:HH21	34:d:39:PRO:HD2	1.78	0.48
5:A:9:G:H2'	5:A:10:U:C6	2.48	0.48
5:A:1605:G:N3	5:A:1605:G:H2'	2.28	0.48
5:A:1865:G:N2	5:A:1868:A:OP2	2.44	0.48
10:F:32:THR:OG1	10:F:157:THR:O	2.29	0.48
31:a:681:U:H2'	31:a:682:G:O4'	2.13	0.48
31:a:1464:C:H2'	31:a:1465:A:H8	1.79	0.48
5:A:1680:G:H2'	5:A:1681:U:C6	2.49	0.48
5:A:2784:C:H2'	5:A:2785:C:C6	2.49	0.48
5:A:2843:U:H2'	5:A:2844:G:O4'	2.14	0.48
31:a:588:U:H2'	31:a:589:A:C8	2.49	0.48
32:b:42:ILE:O	32:b:42:ILE:HG13	2.14	0.48
37:g:98:ALA:O	37:g:102:ARG:HG3	2.14	0.48
5:A:2510:U:H2'	5:A:2511:C:C6	2.49	0.48
7:C:137:ILE:HD11	7:C:167:ARG:HG3	1.95	0.48
27:W:1:MET:O	27:W:2:SER:OG	2.30	0.48
32:b:75:LYS:HD2	32:b:167:ASP:HB2	1.96	0.48
5:A:1464:A:H2'	5:A:1465:A:H8	1.78	0.47
11:G:84:GLU:HB3	11:G:134:LYS:HG2	1.96	0.47
5:A:157:U:H2'	5:A:158:U:C6	2.49	0.47
5:A:2242:G:H2'	5:A:2243:A:C8	2.49	0.47
21:Q:37:ASP:OD1	21:Q:37:ASP:N	2.45	0.47
32:b:210:ARG:H	32:b:210:ARG:HD3	1.79	0.47
42:l:65:SER:OG	42:l:97:THR:OG1	2.22	0.47
10:F:50:LEU:O	10:F:54:VAL:HG13	2.15	0.47
31:a:319:U:H2'	31:a:320:G:O4'	2.14	0.47
31:a:536:A:H2'	31:a:537:G:C8	2.48	0.47
31:a:610:C:OP1	34:d:83:ARG:NH1	2.41	0.47
31:a:1288:C:OP1	37:g:37:SER:OG	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:b:28:LYS:NZ	32:b:196:ASP:OD2	2.28	0.47
33:c:46:LYS:HG2	33:c:47:LEU:HD13	1.95	0.47
5:A:727:G:H5''	5:A:728:A:H5''	1.96	0.47
5:A:2021:C:H2'	5:A:2022:U:C6	2.49	0.47
11:G:13:ASN:OD1	11:G:13:ASN:N	2.48	0.47
32:b:112:SER:O	32:b:115:ARG:HD3	2.14	0.47
36:f:29:ILE:HG22	36:f:34:GLY:HA3	1.96	0.47
41:k:46:SER:HB2	41:k:56:LYS:HG2	1.97	0.47
48:r:32:TYR:CG	48:r:55:LEU:HD21	2.50	0.47
5:A:1481:U:H2'	5:A:1482:C:C6	2.49	0.47
5:A:2853:G:H5'	5:A:2854:U:OP2	2.14	0.47
7:C:107:PRO:HD2	7:C:110:LEU:HD22	1.95	0.47
10:F:57:MET:HE3	10:F:57:MET:N	2.28	0.47
22:R:59:GLU:OE1	22:R:66:VAL:HG22	2.13	0.47
5:A:1481:U:H2'	5:A:1482:C:H6	1.79	0.47
5:A:2510:U:H2'	5:A:2511:C:H6	1.79	0.47
9:E:153:ASP:OD1	9:E:154:GLU:N	2.48	0.47
10:F:162:THR:HG23	10:F:165:GLU:OE2	2.14	0.47
31:a:231:U:H2'	31:a:232:A:C8	2.49	0.47
31:a:552:U:H2'	31:a:553:C:C6	2.49	0.47
31:a:1006:U:H2'	31:a:1007:U:O4'	2.15	0.47
31:a:1059:U:H2'	31:a:1060:C:C6	2.49	0.47
32:b:169:ASP:OD2	32:b:193:SER:OG	2.26	0.47
49:s:43:ASP:N	49:s:43:ASP:OD1	2.48	0.47
51:u:17:ARG:HB3	51:u:21:ARG:NH1	2.28	0.47
5:A:574:U:H2'	5:A:575:G:C8	2.50	0.47
5:A:2302:C:H3'	5:A:2303:G:H5''	1.95	0.47
6:B:31:G:O2'	6:B:32:A:H8	1.97	0.47
10:F:29:PRO:HB3	10:F:160:ALA:HB2	1.96	0.47
27:W:70:ASP:O	27:W:74:GLN:HG3	2.14	0.47
31:a:680:G:N2	41:k:38:GLY:O	2.48	0.47
32:b:185:VAL:HG12	32:b:198:VAL:HG13	1.96	0.47
37:g:26:PHE:HE2	37:g:120:LEU:HD21	1.80	0.47
44:n:15:LYS:HB2	44:n:15:LYS:NZ	2.29	0.47
50:t:16:LYS:HB2	50:t:16:LYS:HE3	1.66	0.47
5:A:592:U:H2'	5:A:593:C:C6	2.49	0.47
5:A:1536:G:H2'	5:A:1537:C:O4'	2.15	0.47
5:A:1590:A:H2'	5:A:1591:C:C6	2.50	0.47
5:A:1723:A:H2'	5:A:1724:C:C6	2.50	0.47
31:a:35:A:H2'	31:a:36:C:H6	1.79	0.47
5:A:226:A:N3	5:A:241:U:O2'	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:1007:U:O4	31:a:1016:G:O6	2.33	0.47
31:a:1011:A:C2	31:a:1216:A:H1'	2.50	0.47
41:k:28:ASN:OD1	41:k:29:THR:N	2.42	0.47
6:B:34:C:H2'	6:B:35:C:H5''	1.97	0.47
10:F:94:ASP:OD1	10:F:95:GLN:N	2.48	0.47
32:b:70:LEU:HD11	32:b:94:VAL:HG23	1.97	0.47
36:f:34:GLY:HA2	36:f:65:GLU:O	2.14	0.47
5:A:1127:U:O2'	5:A:1128:G:H2'	2.14	0.46
5:A:2463:C:H2'	5:A:2464:A:O4'	2.15	0.46
31:a:920:A:H2'	31:a:921:C:C6	2.51	0.46
5:A:97:C:H3'	5:A:98:A:H2'	1.98	0.46
5:A:846:U:H2'	5:A:847:A:C8	2.50	0.46
7:C:133:ARG:NH1	7:C:187:GLU:OE2	2.48	0.46
31:a:37:G:H2'	31:a:38:C:C6	2.50	0.46
36:f:73:GLU:N	36:f:73:GLU:OE1	2.47	0.46
5:A:2060:C:H2'	5:A:2061:C:H6	1.79	0.46
11:G:44:LYS:HA	11:G:44:LYS:CE	2.45	0.46
11:G:47:GLU:HG3	11:G:48:GLY:N	2.30	0.46
31:a:472:A:H2'	31:a:473:U:C6	2.50	0.46
31:a:502:G:H2'	31:a:503:G:C8	2.50	0.46
5:A:161:A:H2'	5:A:162:A:H8	1.81	0.46
5:A:637:U:H2'	5:A:638:C:H6	1.79	0.46
5:A:1403:U:H2'	5:A:1404:G:H8	1.80	0.46
5:A:2341:A:N3	5:A:2377:A:H2'	2.30	0.46
31:a:58:U:H2'	31:a:59:G:H8	1.81	0.46
32:b:70:LEU:HD23	32:b:163:LEU:HD21	1.96	0.46
51:u:17:ARG:HB3	51:u:21:ARG:HH22	1.80	0.46
5:A:353:C:H2'	5:A:354:A:H8	1.80	0.46
5:A:655:U:H2'	5:A:656:U:C6	2.50	0.46
11:G:11:VAL:HG13	11:G:15:VAL:HG23	1.98	0.46
31:a:395:G:H2'	31:a:396:C:C6	2.51	0.46
22:R:10:ALA:HB1	22:R:46:LEU:HD13	1.96	0.46
31:a:185:C:H4'	31:a:186:G:O5'	2.16	0.46
31:a:456:U:H2'	31:a:457:A:H8	1.80	0.46
31:a:577:C:H2'	31:a:578:G:O4'	2.15	0.46
31:a:748:U:H2'	31:a:749:G:O4'	2.16	0.46
31:a:1357:A:OP2	44:n:75:ARG:NH2	2.49	0.46
31:a:1461:U:H2'	31:a:1462:A:C8	2.50	0.46
5:A:279:U:H3	5:A:366:G:H22	1.63	0.46
5:A:2563:G:H2'	5:A:2564:A:C8	2.50	0.46
5:A:2611:U:C2	30:Z:4:GLN:HA	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:1069:G:H2'	31:a:1070:U:C6	2.51	0.46
5:A:580:A:H2'	5:A:581:G:C8	2.50	0.46
5:A:1498:G:H2'	5:A:1499:U:C6	2.51	0.46
7:C:177:ARG:HE	7:C:177:ARG:HB3	1.58	0.46
18:N:35:HIS:ND1	18:N:54:THR:OG1	2.42	0.46
23:S:1:MET:HG2	23:S:44:LYS:HD2	1.98	0.46
31:a:588:U:H2'	31:a:589:A:H8	1.81	0.46
31:a:899:G:H2'	31:a:900:A:H8	1.81	0.46
31:a:1148:A:HO2'	31:a:1149:A:H8	1.62	0.46
34:d:102:ASN:O	34:d:102:ASN:ND2	2.49	0.46
5:A:1569:A:H2'	5:A:1570:A:C8	2.51	0.46
5:A:2242:G:H2'	5:A:2243:A:H8	1.81	0.46
10:F:110:ARG:HB3	10:F:137:VAL:HB	1.98	0.46
22:R:73:THR:HB	22:R:106:LYS:HB2	1.98	0.46
31:a:35:A:H2'	31:a:36:C:C6	2.51	0.46
31:a:590:U:H2'	31:a:591:U:C6	2.52	0.46
31:a:1411:U:H2'	31:a:1412:G:H8	1.80	0.46
32:b:76:ARG:H	32:b:76:ARG:NE	2.13	0.46
5:A:499:G:N1	5:A:502:A:OP2	2.48	0.45
5:A:845:A:OP2	5:A:846:U:H5	1.99	0.45
5:A:2727:G:H2'	5:A:2728:G:C8	2.52	0.45
31:a:295:G:H2'	31:a:296:A:C8	2.50	0.45
31:a:808:C:O2'	31:a:898:A:N1	2.47	0.45
31:a:1092:U:H2'	31:a:1093:C:C6	2.51	0.45
45:o:78:TYR:O	45:o:82:ILE:HG23	2.16	0.45
46:p:87:GLU:HA	46:p:87:GLU:OE2	2.16	0.45
5:A:612:A:H5'	5:A:614:A:C6	2.50	0.45
5:A:687:A:H2'	5:A:688:U:C6	2.51	0.45
5:A:1400:U:H2'	5:A:1401:U:C6	2.51	0.45
5:A:2805:A:H2'	5:A:2806:A:C8	2.51	0.45
8:D:33:ASN:N	8:D:33:ASN:HD22	2.14	0.45
5:A:719:A:H2'	5:A:720:A:C8	2.51	0.45
5:A:2324:A:H2'	5:A:2325:A:H8	1.78	0.45
10:F:72:LYS:HE2	10:F:72:LYS:HB3	1.79	0.45
11:G:54:PRO:HB2	11:G:56:LYS:O	2.17	0.45
31:a:943:A:H2'	31:a:944:G:H8	1.77	0.45
5:A:306:U:H2'	5:A:307:C:C6	2.51	0.45
5:A:1016:U:OP1	5:A:1032:U:O2'	2.30	0.45
5:A:1866:U:H2'	5:A:1867:A:O4'	2.17	0.45
5:A:2793:U:O4	5:A:2797:G:N2	2.34	0.45
11:G:72:LEU:O	11:G:76:VAL:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:474:A:H2'	31:a:475:G:H8	1.81	0.45
5:A:1356:G:H2'	5:A:1357:C:C6	2.52	0.45
5:A:1722:A:H2'	5:A:1723:A:C8	2.51	0.45
27:W:34:HIS:NE2	27:W:56:MET:SD	2.89	0.45
31:a:920:A:H2'	31:a:921:C:H6	1.81	0.45
31:a:1248:A:H2'	31:a:1249:A:C8	2.51	0.45
5:A:740:G:H2'	5:A:741:U:H6	1.81	0.45
5:A:869:U:H2'	5:A:870:U:C6	2.51	0.45
5:A:1194:U:H2'	5:A:1195:C:H6	1.82	0.45
5:A:1722:A:H2'	5:A:1723:A:H8	1.82	0.45
5:A:2187:A:H2'	5:A:2188:G:C8	2.52	0.45
5:A:2469:U:O2	5:A:2469:U:H2'	2.15	0.45
5:A:2586:A:H2'	5:A:2587:C:C6	2.51	0.45
24:T:80:ARG:HB2	24:T:95:LYS:HG3	1.98	0.45
31:a:412:G:H2'	31:a:413:G:H8	1.82	0.45
31:a:1037:A:H2'	31:a:1038:G:H8	1.81	0.45
31:a:1349:C:H2'	31:a:1350:G:C8	2.51	0.45
36:f:98:GLU:H	36:f:98:GLU:CD	2.24	0.45
39:i:55:ALA:HB1	39:i:58:LYS:HB2	1.98	0.45
43:m:68:ASP:OD1	43:m:68:ASP:N	2.49	0.45
10:F:49:LEU:HD23	10:F:49:LEU:H	1.82	0.45
19:O:39:ASP:OD1	19:O:39:ASP:N	2.49	0.45
31:a:1311:C:H2'	31:a:1312:U:H6	1.81	0.45
33:c:131:ARG:O	33:c:135:LYS:HG3	2.17	0.45
5:A:158:U:H2'	5:A:159:G:H8	1.82	0.45
5:A:2312:G:H2'	5:A:2313:C:C6	2.52	0.45
8:D:20:GLY:HA3	19:O:83:VAL:HG13	1.99	0.45
31:a:534:A:H2'	31:a:535:G:H8	1.82	0.45
31:a:1127:A:H2'	31:a:1128:G:H8	1.81	0.45
32:b:225:ALA:HA	32:b:227:LYS:HE2	1.98	0.45
5:A:811:U:H2'	5:A:812:C:C6	2.51	0.45
5:A:997:A:H2'	5:A:998:A:C8	2.52	0.45
6:B:55:A:O2'	10:F:27:GLU:OE2	2.26	0.45
25:U:67:ILE:HD12	25:U:76:VAL:HG21	1.98	0.45
31:a:759:U:H2'	31:a:760:A:C8	2.52	0.45
31:a:905:A:H2'	31:a:906:A:C8	2.50	0.45
5:A:794:C:H2'	5:A:795:U:C6	2.52	0.45
5:A:809:U:H2'	15:K:23:ARG:HA	1.99	0.45
5:A:830:U:H2'	5:A:831:A:H8	1.82	0.45
5:A:1733:U:H3'	5:A:1734:G:C8	2.52	0.45
28:X:12:GLU:HA	28:X:12:GLU:OE1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:X:26:PHE:CE1	28:X:30:MET:HE3	2.51	0.45
31:a:878:G:P	42:l:9:ARG:HH22	2.40	0.45
31:a:1038:G:H2'	31:a:1039:A:C8	2.52	0.45
31:a:1118:U:H2'	31:a:1119:U:C6	2.52	0.45
31:a:1402:G:H2'	31:a:1403:U:H6	1.82	0.45
32:b:128:PHE:CZ	32:b:139:ARG:HB3	2.52	0.45
10:F:47:LYS:HD2	10:F:47:LYS:HA	1.87	0.44
11:G:23:GLN:N	11:G:23:GLN:OE1	2.50	0.44
16:L:48:GLU:OE2	16:L:52:ARG:NH2	2.50	0.44
19:O:65:ARG:NH1	19:O:74:GLU:OE1	2.48	0.44
25:U:68:LYS:HB2	25:U:68:LYS:NZ	2.32	0.44
31:a:1360:A:O2'	31:a:1362:G:N7	2.41	0.44
34:d:158:LYS:O	34:d:161:ILE:HG12	2.18	0.44
5:A:199:G:O2'	5:A:675:A:N1	2.46	0.44
5:A:2683:U:H2'	5:A:2684:G:O4'	2.16	0.44
13:I:31:GLU:HG2	13:I:142:ILE:HB	1.99	0.44
31:a:908:U:H2'	31:a:909:C:C6	2.52	0.44
32:b:209:ILE:HA	32:b:212:VAL:HG12	1.98	0.44
34:d:61:GLN:HB3	34:d:65:ARG:NH1	2.33	0.44
14:J:63:VAL:HG12	14:J:106:LEU:HD11	1.98	0.44
31:a:506:A:N3	31:a:540:U:O2'	2.47	0.44
31:a:534:A:H2'	31:a:535:G:C8	2.52	0.44
31:a:1374:A:OP1	37:g:92:ARG:NH1	2.47	0.44
32:b:198:VAL:HB	32:b:201:VAL:HG22	1.98	0.44
32:b:224:LEU:O	32:b:227:LYS:HG3	2.18	0.44
34:d:192:ASP:OD1	34:d:192:ASP:N	2.50	0.44
37:g:17:LYS:HE2	37:g:18:PHE:CE1	2.53	0.44
41:k:70:GLY:O	41:k:104:TYR:OH	2.27	0.44
5:A:9:G:H2'	5:A:10:U:H6	1.82	0.44
5:A:976:A:H5''	5:A:977:A:H5''	1.98	0.44
5:A:1647:G:O2'	17:M:106:ASP:OD2	2.26	0.44
5:A:2369:A:H2'	5:A:2370:C:C6	2.53	0.44
5:A:2841:U:H5''	19:O:55:ASN:O	2.17	0.44
31:a:1521:C:H2'	31:a:1522:G:C8	2.53	0.44
34:d:67:TYR:OH	34:d:97:GLU:OE2	2.31	0.44
34:d:89:GLY:HA3	34:d:199:GLU:HG3	2.00	0.44
36:f:29:ILE:HD11	36:f:74:LEU:HD11	1.98	0.44
49:s:62:VAL:HA	49:s:66:MET:CE	2.47	0.44
51:u:4:VAL:HG21	51:u:19:PHE:HA	2.00	0.44
5:A:365:U:H1'	5:A:366:G:OP2	2.17	0.44
5:A:1050:U:O4	5:A:1051:A:N6	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1437:U:H2'	5:A:1438:C:C6	2.53	0.44
5:A:2212:G:H2'	5:A:2213:G:H8	1.83	0.44
5:A:2308:U:O3'	10:F:68:THR:HG21	2.18	0.44
5:A:2641:U:H4'	5:A:2728:G:O2'	2.18	0.44
31:a:232:A:H2'	31:a:233:A:H8	1.83	0.44
31:a:521:G:H2'	31:a:522:C:C6	2.51	0.44
33:c:27:LYS:HD3	33:c:27:LYS:N	2.33	0.44
36:f:56:LYS:HB2	36:f:56:LYS:HE3	1.89	0.44
37:g:113:GLU:HB2	37:g:119:ARG:HG3	1.98	0.44
34:d:11:LEU:HG	34:d:65:ARG:NE	2.31	0.44
37:g:17:LYS:HG2	37:g:18:PHE:CD1	2.53	0.44
39:i:110:GLU:OE2	39:i:113:LYS:NZ	2.44	0.44
51:u:28:VAL:O	51:u:32:VAL:HG23	2.18	0.44
5:A:347:A:H1'	5:A:348:A:C2	2.52	0.44
5:A:678:A:H2'	5:A:679:G:C8	2.53	0.44
5:A:2303:G:H8	5:A:2303:G:OP1	2.00	0.44
31:a:91:G:H2'	31:a:92:G:C8	2.53	0.44
31:a:367:A:H2'	31:a:368:C:O4'	2.18	0.44
31:a:982:C:H2'	31:a:983:U:C6	2.53	0.44
31:a:1005:U:H2'	31:a:1006:U:C6	2.53	0.44
31:a:1038:G:H2'	31:a:1039:A:H8	1.82	0.44
37:g:26:PHE:CE2	37:g:120:LEU:HD21	2.53	0.44
5:A:1563:C:O2	5:A:1564:A:O2'	2.25	0.44
5:A:1577:A:H2'	5:A:1578:A:H8	1.83	0.44
5:A:2830:G:H2'	5:A:2875:A:H61	1.82	0.44
31:a:435:U:C2	31:a:436:A:C8	3.05	0.44
31:a:1401:C:H2'	31:a:1402:G:C8	2.53	0.44
33:c:14:VAL:O	33:c:211:MET:HG2	2.18	0.44
39:i:7:THR:O	39:i:83:ARG:HD2	2.18	0.44
40:j:29:ALA:O	40:j:32:THR:HG22	2.17	0.44
5:A:390:A:H1'	5:A:410:G:O4'	2.18	0.43
8:D:43:THR:HG23	8:D:44:ASP:OD2	2.18	0.43
10:F:43:ALA:HA	10:F:49:LEU:HD21	2.00	0.43
10:F:65:PRO:HA	10:F:89:VAL:HG12	1.98	0.43
25:U:76:VAL:HG12	25:U:97:ARG:HA	2.00	0.43
31:a:185:C:H1'	31:a:186:G:OP2	2.17	0.43
31:a:380:C:H2'	31:a:381:C:H6	1.83	0.43
31:a:742:U:OP1	31:a:848:U:O2'	2.28	0.43
31:a:1393:A:H4'	31:a:1394:C:H5''	2.00	0.43
5:A:1046:C:C2	5:A:1047:A:C8	3.06	0.43
5:A:1489:A:H2'	5:A:1490:A:C8	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2034:G:H2'	5:A:2035:U:O4'	2.18	0.43
26:V:11:LYS:HB3	26:V:11:LYS:HE2	1.50	0.43
31:a:976:C:O2	44:n:59:ARG:NH1	2.50	0.43
31:a:1235:A:H2	31:a:1238:G:N3	2.16	0.43
5:A:1104:G:N2	5:A:1105:U:O4	2.40	0.43
5:A:1543:A:H3'	5:A:1544:G:H8	1.84	0.43
11:G:27:LYS:HE3	11:G:27:LYS:HB3	1.77	0.43
26:V:46:HIS:CD2	26:V:77:ARG:HD2	2.53	0.43
36:f:1:MET:HE1	36:f:33:ASP:HB3	1.99	0.43
37:g:72:MET:SD	37:g:72:MET:N	2.91	0.43
40:j:47:GLU:O	40:j:66:GLU:HA	2.18	0.43
41:k:36:ARG:HB2	41:k:37:GLN:NE2	2.34	0.43
5:A:369:G:O2'	5:A:423:G:OP1	2.32	0.43
5:A:1412:C:H2'	5:A:1413:G:O4'	2.18	0.43
5:A:2840:A:O2'	19:O:2:SER:N	2.41	0.43
6:B:60:U:H2'	6:B:61:C:H6	1.84	0.43
10:F:51:ASP:OD1	10:F:51:ASP:N	2.52	0.43
11:G:84:GLU:HA	11:G:133:LEU:O	2.18	0.43
31:a:78:G:H2'	31:a:79:U:C6	2.52	0.43
31:a:536:A:H2'	31:a:537:G:H8	1.84	0.43
5:A:707:U:H2'	5:A:708:U:C6	2.53	0.43
5:A:1273:C:H2'	5:A:1274:G:H8	1.83	0.43
6:B:22:G:N7	6:B:54:G:H2'	2.34	0.43
6:B:43:A:C4	6:B:44:A:C8	3.05	0.43
11:G:17:VAL:HG11	11:G:50:LEU:HD21	2.00	0.43
18:N:78:ALA:HB2	18:N:109:ALA:HA	2.01	0.43
31:a:74:G:N2	31:a:93:A:N1	2.49	0.43
31:a:888:U:OP2	31:a:903:A:N6	2.50	0.43
32:b:22:THR:HG22	32:b:41:HIS:CE1	2.54	0.43
34:d:36:ASN:HA	34:d:46:ARG:HD3	2.00	0.43
37:g:107:ALA:HB1	37:g:133:ALA:HB3	2.00	0.43
5:A:292:U:H2'	5:A:293:U:C6	2.53	0.43
5:A:418:U:H2'	5:A:419:C:H6	1.82	0.43
5:A:596:U:H2'	5:A:597:A:H8	1.83	0.43
5:A:1730:U:H2'	5:A:1731:C:H6	1.82	0.43
5:A:2457:A:H2'	5:A:2458:C:C6	2.53	0.43
5:A:2696:A:H2'	5:A:2697:C:C6	2.53	0.43
31:a:23:G:H2'	31:a:24:G:C8	2.53	0.43
31:a:202:U:H2'	31:a:203:C:C6	2.54	0.43
31:a:1425:A:H2'	31:a:1426:C:C6	2.54	0.43
32:b:112:SER:HA	32:b:115:ARG:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:k:80:ASN:HB2	41:k:107:ASN:OD1	2.18	0.43
45:o:14:LYS:HD3	45:o:15:PHE:CE2	2.54	0.43
51:u:13:ASP:O	51:u:17:ARG:HG3	2.18	0.43
5:A:521:G:H2'	5:A:522:C:C6	2.54	0.43
5:A:2645:C:H2'	5:A:2646:U:H6	1.83	0.43
31:a:1247:A:H2'	31:a:1248:A:C8	2.54	0.43
31:a:1433:U:H2'	31:a:1434:A:H8	1.83	0.43
31:a:1464:C:H2'	31:a:1465:A:C8	2.54	0.43
34:d:97:GLU:HA	34:d:102:ASN:OD1	2.18	0.43
5:A:844:A:H4'	5:A:845:A:O5'	2.18	0.43
6:B:66:C:H2'	6:B:67:G:O4'	2.18	0.43
10:F:135:GLN:NE2	10:F:149:ILE:HA	2.34	0.43
31:a:37:G:H2'	31:a:38:C:H6	1.84	0.43
31:a:693:A:H2'	31:a:694:U:H6	1.84	0.43
31:a:1404:C:C2	31:a:1405:A:C8	3.06	0.43
31:a:1504:A:H2'	31:a:1505:G:C8	2.54	0.43
5:A:142:A:H2'	5:A:143:C:C6	2.53	0.43
5:A:189:A:H2'	5:A:190:C:C6	2.54	0.43
5:A:611:U:H5'	5:A:612:A:C8	2.53	0.43
5:A:1297:A:OP2	5:A:1605:G:O2'	2.29	0.43
5:A:1729:U:H2'	5:A:1730:U:C6	2.53	0.43
5:A:2696:A:H2'	5:A:2697:C:H6	1.83	0.43
20:P:58:ARG:HA	20:P:61:TRP:CE3	2.54	0.43
31:a:424:G:H5''	34:d:10:LYS:HD2	2.00	0.43
31:a:470:G:H2'	31:a:471:G:C8	2.53	0.43
31:a:470:G:H2'	31:a:471:G:H8	1.83	0.43
31:a:1394:C:OP2	35:e:28:ARG:NH2	2.35	0.43
31:a:1399:4OC:O5'	31:a:1399:4OC:H6	2.19	0.43
36:f:19:VAL:O	36:f:23:GLU:HG2	2.19	0.43
5:A:215:C:H2'	5:A:216:C:H6	1.83	0.43
5:A:1923:A:H2'	5:A:1924:A:C8	2.54	0.43
5:A:2451:G:H2'	5:A:2452:C:C6	2.54	0.43
19:O:28:THR:CG2	19:O:91:ARG:HB3	2.48	0.43
23:S:5:ARG:O	23:S:9:VAL:HG23	2.19	0.43
31:a:436:A:C4	31:a:437:A:C8	3.07	0.43
32:b:145:LYS:O	32:b:149:SER:OG	2.29	0.43
34:d:22:LYS:HD2	34:d:31:LYS:HE2	2.00	0.43
5:A:148:A:OP1	23:S:44:LYS:NZ	2.33	0.42
5:A:568:G:H2'	5:A:2026:6MZ:N7	2.33	0.42
5:A:1577:A:H2'	5:A:1578:A:C8	2.54	0.42
5:A:2288:G:H2'	5:A:2289:C:C6	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2674:A:H2'	5:A:2675:A:H8	1.84	0.42
10:F:26:MET:HE3	10:F:26:MET:HA	2.01	0.42
11:G:33:LEU:HD13	11:G:75:LEU:HD22	1.99	0.42
19:O:2:SER:O	19:O:2:SER:OG	2.25	0.42
31:a:734:A:H2'	31:a:735:U:H6	1.84	0.42
46:p:22:ILE:HG12	46:p:39:VAL:HG22	2.01	0.42
5:A:1480:A:H2'	5:A:1481:U:C6	2.55	0.42
5:A:1724:C:O2'	5:A:1725:U:H5'	2.18	0.42
5:A:837:U:H2'	5:A:838:C:C6	2.54	0.42
5:A:1036:A:N1	5:A:1113:G:N2	2.53	0.42
5:A:2247:OMG:H1'	5:A:2247:OMG:HM23	1.72	0.42
6:B:16:A:H2'	6:B:17:A:H8	1.84	0.42
8:D:81:LYS:HG3	8:D:82:GLU:N	2.32	0.42
31:a:200:G:C8	31:a:461:A:N1	2.87	0.42
31:a:403:U:O2'	34:d:115:GLU:HG3	2.19	0.42
31:a:1157:G:H1	31:a:1173:A:N6	2.17	0.42
31:a:1510:A:H2'	31:a:1511:G:C8	2.54	0.42
5:A:1935:5MU:OP1	5:A:2600:U:O2'	2.34	0.42
5:A:2550:U:H2'	5:A:2551:U:C6	2.54	0.42
6:B:46:U:H2'	6:B:47:C:C6	2.53	0.42
15:K:2:THR:N	15:K:7:GLU:OE1	2.53	0.42
19:O:90:LYS:HE3	19:O:90:LYS:HB3	1.78	0.42
31:a:454:U:H2'	31:a:455:C:C6	2.54	0.42
31:a:1493:C:H2'	31:a:1494:G:O4'	2.19	0.42
34:d:170:PRO:HB3	34:d:172:TRP:CH2	2.54	0.42
51:u:35:ARG:HA	51:u:35:ARG:HD3	1.74	0.42
5:A:347:A:H1'	5:A:348:A:H2	1.85	0.42
5:A:568:G:H2'	5:A:2026:6MZ:C8	2.50	0.42
5:A:2743:G:O6	5:A:2751:C:H5''	2.20	0.42
31:a:200:G:C4	31:a:201:A:C8	3.07	0.42
31:a:385:A:H3'	31:a:386:U:H6	1.84	0.42
31:a:673:A:H2'	31:a:674:U:H6	1.84	0.42
31:a:1144:C:O2'	39:i:5:TYR:OH	2.28	0.42
31:a:1157:G:H1	31:a:1173:A:H61	1.68	0.42
31:a:1383:G:H2'	31:a:1384:G:H8	1.83	0.42
33:c:10:ILE:HG23	33:c:11:ARG:HG3	2.01	0.42
33:c:175:LEU:HD23	33:c:175:LEU:HA	1.88	0.42
34:d:16:GLY:O	34:d:46:ARG:NH2	2.53	0.42
36:f:10:VAL:HG11	36:f:18:VAL:HG12	2.01	0.42
47:q:9:LEU:HB3	47:q:26:ILE:HD12	2.02	0.42
5:A:498:U:H2'	5:A:499:G:O4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:596:U:H2'	5:A:597:A:C8	2.55	0.42
5:A:1193:U:C2	5:A:1194:U:C5	3.08	0.42
5:A:1805:A:H2'	5:A:1806:A:C8	2.54	0.42
5:A:2325:A:H2'	5:A:2326:G:H8	1.84	0.42
31:a:200:G:H2'	31:a:201:A:C8	2.53	0.42
31:a:251:G:H2'	31:a:252:U:C6	2.55	0.42
31:a:525:C:N4	42:l:46:ASN:OD1	2.47	0.42
32:b:7:SER:O	32:b:8:MET:HB2	2.19	0.42
32:b:138:GLU:OE2	32:b:138:GLU:N	2.52	0.42
40:j:80:THR:HG22	40:j:81:ASP:H	1.85	0.42
5:A:145:U:H2'	5:A:146:U:C6	2.54	0.42
5:A:1478:G:H2'	5:A:1479:U:C6	2.55	0.42
5:A:1681:U:H2'	5:A:1682:A:C8	2.55	0.42
5:A:2269:A:H2'	5:A:2270:A:C8	2.54	0.42
5:A:2533:U:H2'	5:A:2534:C:H6	1.83	0.42
10:F:94:ASP:OD1	10:F:94:ASP:C	2.61	0.42
24:T:6:LYS:O	24:T:24:VAL:HG22	2.19	0.42
24:T:79:ASP:OD2	24:T:96:SER:OG	2.26	0.42
31:a:1326:A:OP1	43:m:29:THR:OG1	2.35	0.42
45:o:17:ARG:HG2	45:o:17:ARG:HH11	1.85	0.42
5:A:1165:U:H2'	5:A:1166:A:H8	1.85	0.42
5:A:2302:C:C3'	5:A:2303:G:H5''	2.50	0.42
6:B:35:C:O2	18:N:99:HIS:NE2	2.37	0.42
11:G:154:PRO:HD3	11:G:162:VAL:O	2.20	0.42
37:g:44:TYR:O	37:g:48:GLU:HG3	2.18	0.42
45:o:17:ARG:HG2	45:o:17:ARG:NH1	2.34	0.42
5:A:358:A:H2'	5:A:359:U:C6	2.55	0.42
5:A:665:U:H2'	5:A:666:A:O4'	2.20	0.42
10:F:74:ILE:HG22	10:F:77:PHE:H	1.85	0.42
31:a:754:U:H2'	31:a:755:G:O4'	2.20	0.42
31:a:818:G:H2'	31:a:819:U:H6	1.84	0.42
31:a:1001:A:C5	31:a:1023:G:H1'	2.55	0.42
45:o:53:ARG:O	45:o:57:ILE:HG12	2.20	0.42
48:r:28:THR:HA	48:r:31:GLN:HG3	2.01	0.42
5:A:1165:U:H2'	5:A:1166:A:C8	2.55	0.42
25:U:34:ILE:HD11	25:U:67:ILE:HD13	2.02	0.42
31:a:69:C:H2'	31:a:70:G:C8	2.55	0.42
31:a:1092:U:P	31:a:1105:G:H1	2.42	0.42
32:b:14:ALA:O	32:b:210:ARG:NE	2.53	0.42
41:k:114:PRO:O	41:k:115:ILE:HD13	2.19	0.42
5:A:284:U:H3	5:A:360:A:N6	2.14	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2283:A:C5	5:A:2285:G:C8	3.08	0.41
5:A:2373:A:H2'	5:A:2374:A:C8	2.55	0.41
31:a:331:C:H2'	31:a:332:A:H8	1.84	0.41
31:a:1115:U:H1'	31:a:1176:A:C5	2.55	0.41
34:d:4:TYR:CD1	34:d:4:TYR:C	2.97	0.41
37:g:49:ARG:HE	37:g:121:ALA:CB	2.33	0.41
5:A:2212:G:H2'	5:A:2213:G:C8	2.55	0.41
26:V:37:ILE:HG22	26:V:38:VAL:HG23	2.01	0.41
31:a:154:C:N4	31:a:155:G:O6	2.52	0.41
31:a:590:U:H2'	31:a:591:U:H6	1.85	0.41
31:a:715:A:H5'	41:k:118:ASN:CG	2.44	0.41
36:f:42:TRP:HZ2	36:f:61:LEU:HD22	1.85	0.41
43:m:106:ALA:HB3	43:m:110:LYS:HD3	2.01	0.41
46:p:74:ARG:HD2	46:p:74:ARG:HA	1.80	0.41
5:A:37:G:H2'	5:A:38:C:C6	2.55	0.41
5:A:291:G:H2'	5:A:292:U:C6	2.55	0.41
5:A:1310:C:H2'	5:A:1311:A:H8	1.85	0.41
5:A:1311:A:H2'	5:A:1312:G:H8	1.85	0.41
5:A:1479:U:H2'	5:A:1480:A:C8	2.53	0.41
5:A:2448:C:H2'	5:A:2449:A:C8	2.55	0.41
10:F:23:LYS:H	10:F:23:LYS:HD2	1.84	0.41
13:I:98:GLU:CD	13:I:98:GLU:H	2.28	0.41
18:N:98:TYR:CE2	18:N:103:LYS:HG3	2.55	0.41
30:Z:52:GLN:OE1	30:Z:53:LEU:N	2.53	0.41
34:d:36:ASN:HA	34:d:46:ARG:HH11	1.86	0.41
40:j:6:ILE:HB	40:j:76:ILE:HB	2.02	0.41
5:A:324:A:OP2	9:E:162:ASN:HB2	2.20	0.41
5:A:1198:U:OP2	5:A:1199:A:O2'	2.32	0.41
5:A:1523:A:H2'	5:A:1524:A:C8	2.55	0.41
5:A:1928:A:H2'	5:A:1929:G:O4'	2.20	0.41
5:A:2288:G:H2'	5:A:2289:C:H6	1.85	0.41
5:A:2456:U:C2	5:A:2457:A:C8	3.09	0.41
5:A:2853:G:N2	5:A:2856:A:OP2	2.46	0.41
31:a:18:A:H8	31:a:1077:A:O2'	2.03	0.41
31:a:79:U:H2'	31:a:80:A:C8	2.55	0.41
31:a:180:U:C2	31:a:181:C:C5	3.09	0.41
31:a:994:U:H2'	31:a:995:A:C8	2.49	0.41
31:a:1146:U:H2'	31:a:1147:U:C6	2.55	0.41
31:a:1304:U:H2'	31:a:1305:U:C6	2.55	0.41
32:b:17:HIS:HB3	32:b:45:LEU:HD21	2.01	0.41
33:c:31:GLU:H	33:c:31:GLU:HG3	1.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:k:35:ASP:HB3	41:k:41:LEU:HD11	2.02	0.41
5:A:968:C:H2'	5:A:969:A:O4'	2.20	0.41
5:A:1314:C:O2'	5:A:1315:C:H5'	2.19	0.41
5:A:1665:G:O2'	5:A:1987:U:O4	2.35	0.41
5:A:2314:G:H2'	5:A:2315:U:O4'	2.20	0.41
23:S:4:GLU:OE1	28:X:22:GLN:NE2	2.54	0.41
31:a:454:U:H2'	31:a:455:C:H6	1.85	0.41
31:a:734:A:H2'	31:a:735:U:C6	2.55	0.41
31:a:818:G:H2'	31:a:819:U:C6	2.55	0.41
31:a:1093:C:H2'	31:a:1094:C:H6	1.86	0.41
31:a:1323:U:H2'	31:a:1324:C:H6	1.86	0.41
31:a:1488:G:H2'	31:a:1489:A:H8	1.85	0.41
36:f:6:ILE:HG12	36:f:89:ILE:HG12	2.02	0.41
36:f:18:VAL:HG11	36:f:58:HIS:HD2	1.86	0.41
36:f:30:LYS:HE3	36:f:30:LYS:HB2	1.75	0.41
44:n:19:LYS:HD3	44:n:20:TYR:CE2	2.55	0.41
5:A:1045:A:H2'	5:A:1045:A:N3	2.35	0.41
5:A:1437:U:H2'	5:A:1438:C:H6	1.84	0.41
5:A:2262:A:H4'	5:A:2263:A:N3	2.36	0.41
6:B:30:U:C4	6:B:49:G:N1	2.89	0.41
7:C:270:ASP:OD1	7:C:274:LYS:HB3	2.21	0.41
10:F:55:ALA:O	10:F:59:LEU:HG	2.20	0.41
13:I:34:ARG:HG3	13:I:39:LYS:HB2	2.01	0.41
31:a:572:G:O2'	31:a:818:G:OP2	2.34	0.41
31:a:887:G:H1'	31:a:903:A:N6	2.36	0.41
31:a:1344:G:N7	39:i:11:LYS:HE3	2.36	0.41
34:d:102:ASN:ND2	34:d:102:ASN:C	2.78	0.41
35:e:55:VAL:O	35:e:59:ILE:HG13	2.21	0.41
36:f:38:ARG:NH1	36:f:100:SER:HB3	2.36	0.41
48:r:25:ASP:O	48:r:29:LEU:HG	2.19	0.41
5:A:907:A:H2'	5:A:910:C:C5	2.55	0.41
5:A:1389:U:H2'	5:A:1390:A:O4'	2.21	0.41
5:A:2836:U:H2'	5:A:2837:U:C6	2.56	0.41
5:A:2883:C:H2'	5:A:2884:U:C6	2.56	0.41
6:B:60:U:H2'	6:B:61:C:C6	2.56	0.41
11:G:69:ARG:HH12	11:G:73:ASN:HB2	1.85	0.41
31:a:1023:G:N3	31:a:1023:G:H2'	2.35	0.41
41:k:74:LEU:HA	41:k:74:LEU:HD23	1.82	0.41
5:A:1316:A:C4	5:A:1317:A:C8	3.09	0.41
5:A:2539:G:H2'	5:A:2540:G:C8	2.56	0.41
31:a:842:A:H2'	31:a:843:G:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:1117:C:H2'	31:a:1118:U:H6	1.86	0.41
32:b:78:ALA:O	32:b:82:ILE:HG22	2.21	0.41
34:d:64:ARG:HE	34:d:64:ARG:HB3	1.70	0.41
5:A:101:U:H2'	5:A:102:A:C8	2.56	0.41
5:A:177:G:H2'	5:A:178:U:C6	2.56	0.41
5:A:234:A:C2	5:A:2403:A:H1'	2.56	0.41
5:A:254:G:H4'	5:A:385:G:C5	2.56	0.41
8:D:184:ASP:OD2	8:D:187:ARG:HD2	2.20	0.41
10:F:50:LEU:HD11	10:F:67:VAL:HG13	2.02	0.41
28:X:40:SER:O	28:X:43:VAL:HG22	2.21	0.41
31:a:207:G:O2'	31:a:208:G:O5'	2.39	0.41
31:a:776:C:H2'	31:a:777:A:O4'	2.20	0.41
31:a:941:G:N1	31:a:1335:G:OP2	2.51	0.41
31:a:964:5MC:OP2	31:a:965:A:O2'	2.38	0.41
31:a:1092:U:H2'	31:a:1093:C:H6	1.86	0.41
31:a:1173:A:H2'	31:a:1174:G:C8	2.56	0.41
31:a:1433:U:H2'	31:a:1434:A:C8	2.56	0.41
31:a:1439:G:H2'	31:a:1440:C:C6	2.56	0.41
35:e:164:GLN:CD	38:h:115:ARG:HD3	2.45	0.41
37:g:53:LYS:CE	37:g:54:ASN:HD22	2.30	0.41
5:A:189:A:H2'	5:A:190:C:H6	1.85	0.41
5:A:1403:U:H2'	5:A:1404:G:C8	2.55	0.41
5:A:1509:U:H2'	5:A:1510:G:O4'	2.21	0.41
5:A:2553:G:H2'	5:A:2554:C:C6	2.56	0.41
10:F:110:ARG:CZ	10:F:110:ARG:HB2	2.51	0.41
31:a:78:G:H2'	31:a:79:U:H6	1.86	0.41
31:a:1005:U:H2'	31:a:1006:U:H6	1.86	0.41
31:a:1141:G:N2	31:a:1143:A:H62	2.19	0.41
31:a:1345:U:H4'	39:i:120:ARG:HG3	2.03	0.41
32:b:9:ARG:HH22	32:b:13:GLN:HE21	1.69	0.41
32:b:112:SER:HB3	32:b:150:LEU:HD21	2.03	0.41
34:d:72:ARG:HD3	34:d:72:ARG:HA	1.85	0.41
37:g:131:LYS:HB3	37:g:131:LYS:HE3	1.81	0.41
41:k:83:VAL:HG11	41:k:96:VAL:HG12	2.03	0.41
5:A:12:A:H2'	5:A:13:A:H8	1.84	0.40
5:A:1247:G:N2	20:P:33:ARG:HB3	2.35	0.40
5:A:1537:C:H3'	5:A:1538:A:H8	1.86	0.40
7:C:268:ILE:H	7:C:268:ILE:HG13	1.70	0.40
31:a:406:G:OP2	34:d:31:LYS:NZ	2.46	0.40
31:a:1124:G:H5'	31:a:1277:A:O2'	2.20	0.40
37:g:132:GLY:O	37:g:135:ILE:HD12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:r:26:ILE:CG2	48:r:30:LYS:HE3	2.51	0.40
1:0:40:ARG:HG2	1:0:40:ARG:NH1	2.36	0.40
5:A:2791:C:H2'	5:A:2792:U:C6	2.56	0.40
9:E:193:LYS:HA	9:E:193:LYS:HD2	1.77	0.40
31:a:1030:G:H2'	31:a:1031:G:O4'	2.21	0.40
31:a:1162:U:H3	31:a:1168:A:N6	2.11	0.40
31:a:1305:U:H2'	31:a:1306:G:H8	1.87	0.40
32:b:117:LYS:HE3	32:b:154:LYS:HD3	2.02	0.40
34:d:44:GLN:OE1	34:d:44:GLN:HA	2.22	0.40
34:d:196:GLU:CD	34:d:196:GLU:H	2.29	0.40
36:f:37:HIS:HB3	36:f:97:THR:HG22	2.03	0.40
5:A:1025:A:N6	5:A:1122:G:H2'	2.36	0.40
5:A:1730:U:H2'	5:A:1731:C:C6	2.55	0.40
5:A:2295:G:C2	5:A:2314:G:N2	2.89	0.40
5:A:2509:A:H2'	5:A:2510:U:C6	2.56	0.40
10:F:71:ARG:O	10:F:72:LYS:HB3	2.22	0.40
14:J:12:ASP:OD1	14:J:12:ASP:C	2.63	0.40
35:e:161:GLU:H	35:e:161:GLU:CD	2.30	0.40
41:k:61:ALA:HA	41:k:64:VAL:HG22	2.03	0.40
42:l:57:LEU:HD11	42:l:82:ILE:HD11	2.03	0.40
5:A:319:A:H2'	5:A:320:A:H8	1.87	0.40
5:A:1317:A:C5	5:A:1318:C:C5	3.09	0.40
5:A:1962:A:N3	5:A:2588:G:O2'	2.42	0.40
5:A:2753:A:H2'	5:A:2754:A:H5''	2.03	0.40
15:K:112:ILE:HB	15:K:129:LEU:HD23	2.02	0.40
17:M:114:GLU:HG2	17:M:115:LEU:O	2.22	0.40
31:a:199:G:O2'	31:a:200:G:H8	2.04	0.40
40:j:51:VAL:HG13	44:n:81:ARG:HB2	2.03	0.40
41:k:33:ILE:HD13	41:k:33:ILE:HA	1.93	0.40
42:l:74:LEU:HD11	42:l:104:CYS:SG	2.61	0.40
5:A:1498:G:H2'	5:A:1499:U:H6	1.87	0.40
5:A:2211:C:H2'	5:A:2212:G:H8	1.87	0.40
10:F:22:ILE:CG2	10:F:27:GLU:HB2	2.52	0.40
16:L:78:PRO:O	16:L:79:LEU:HB3	2.21	0.40
16:L:91:GLU:HB3	16:L:92:TYR:HD1	1.86	0.40
18:N:36:ILE:HG22	18:N:54:THR:HG23	2.03	0.40
21:Q:26:LYS:HA	21:Q:26:LYS:HD3	1.88	0.40
31:a:380:C:H2'	31:a:381:C:C6	2.55	0.40
31:a:1116:C:H2'	31:a:1117:C:H6	1.86	0.40
32:b:83:ARG:NH1	32:b:93:TYR:HE2	2.19	0.40
39:i:34:GLU:HA	39:i:43:ARG:HH11	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	49/51 (96%)	49 (100%)	0	0	100	100
2	1	42/44 (96%)	42 (100%)	0	0	100	100
3	2	61/64 (95%)	60 (98%)	1 (2%)	0	100	100
4	3	36/38 (95%)	36 (100%)	0	0	100	100
7	C	269/274 (98%)	262 (97%)	6 (2%)	1 (0%)	30	33
8	D	209/212 (99%)	202 (97%)	7 (3%)	0	100	100
9	E	198/200 (99%)	198 (100%)	0	0	100	100
10	F	172/178 (97%)	156 (91%)	14 (8%)	2 (1%)	10	8
11	G	172/177 (97%)	167 (97%)	4 (2%)	1 (1%)	21	22
12	H	58/148 (39%)	55 (95%)	3 (5%)	0	100	100
13	I	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
14	J	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
15	K	142/146 (97%)	139 (98%)	3 (2%)	0	100	100
16	L	135/137 (98%)	131 (97%)	4 (3%)	0	100	100
17	M	117/125 (94%)	117 (100%)	0	0	100	100
18	N	113/116 (97%)	112 (99%)	1 (1%)	0	100	100
19	O	115/122 (94%)	114 (99%)	1 (1%)	0	100	100
20	P	115/119 (97%)	115 (100%)	0	0	100	100
21	Q	101/103 (98%)	99 (98%)	1 (1%)	1 (1%)	12	11
22	R	107/109 (98%)	106 (99%)	1 (1%)	0	100	100
23	S	89/106 (84%)	88 (99%)	1 (1%)	0	100	100
24	T	101/105 (96%)	98 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	U	95/98 (97%)	95 (100%)	0	0	100	100
26	V	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
27	W	76/78 (97%)	75 (99%)	1 (1%)	0	100	100
28	X	58/65 (89%)	57 (98%)	1 (2%)	0	100	100
29	Y	55/58 (95%)	55 (100%)	0	0	100	100
30	Z	52/61 (85%)	51 (98%)	1 (2%)	0	100	100
32	b	223/250 (89%)	211 (95%)	10 (4%)	2 (1%)	14	13
33	c	213/250 (85%)	207 (97%)	6 (3%)	0	100	100
34	d	205/208 (99%)	202 (98%)	3 (2%)	0	100	100
35	e	153/165 (93%)	153 (100%)	0	0	100	100
36	f	102/127 (80%)	97 (95%)	3 (3%)	2 (2%)	6	3
37	g	132/156 (85%)	129 (98%)	2 (2%)	1 (1%)	16	15
38	h	128/131 (98%)	125 (98%)	3 (2%)	0	100	100
39	i	124/128 (97%)	120 (97%)	4 (3%)	0	100	100
40	j	98/103 (95%)	95 (97%)	3 (3%)	0	100	100
41	k	115/128 (90%)	110 (96%)	5 (4%)	0	100	100
42	l	120/124 (97%)	114 (95%)	6 (5%)	0	100	100
43	m	113/118 (96%)	109 (96%)	4 (4%)	0	100	100
44	n	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
45	o	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
46	p	80/101 (79%)	80 (100%)	0	0	100	100
47	q	77/85 (91%)	77 (100%)	0	0	100	100
48	r	50/75 (67%)	50 (100%)	0	0	100	100
49	s	80/91 (88%)	77 (96%)	3 (4%)	0	100	100
50	t	84/88 (96%)	84 (100%)	0	0	100	100
51	u	60/71 (84%)	59 (98%)	1 (2%)	0	100	100
All	All	5412/5872 (92%)	5286 (98%)	116 (2%)	10 (0%)	44	50

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	C	272	ARG
10	F	137	VAL

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Mol	Chain	Res	Type
32	b	8	MET
36	f	33	ASP
37	g	3	ARG
10	F	5	LYS
11	G	12	PRO
32	b	7	SER
36	f	94	HIS
21	Q	52	PRO

5.3.2 Protein sidechains [i](#)

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	0	47/47 (100%)	46 (98%)	1 (2%)	47	61
2	1	36/36 (100%)	36 (100%)	0	100	100
3	2	52/53 (98%)	52 (100%)	0	100	100
4	3	33/33 (100%)	33 (100%)	0	100	100
7	C	217/220 (99%)	214 (99%)	3 (1%)	59	73
8	D	166/167 (99%)	165 (99%)	1 (1%)	78	88
9	E	155/155 (100%)	151 (97%)	4 (3%)	40	53
10	F	144/147 (98%)	138 (96%)	6 (4%)	26	34
11	G	139/142 (98%)	133 (96%)	6 (4%)	26	33
12	H	45/112 (40%)	45 (100%)	0	100	100
13	I	118/118 (100%)	117 (99%)	1 (1%)	73	84
14	J	103/103 (100%)	103 (100%)	0	100	100
15	K	106/108 (98%)	105 (99%)	1 (1%)	70	82
16	L	113/113 (100%)	111 (98%)	2 (2%)	51	66
17	M	96/101 (95%)	96 (100%)	0	100	100
18	N	84/85 (99%)	81 (96%)	3 (4%)	31	40
19	O	99/102 (97%)	98 (99%)	1 (1%)	68	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	P	85/86 (99%)	85 (100%)	0	100	100
21	Q	84/84 (100%)	81 (96%)	3 (4%)	31	40
22	R	88/88 (100%)	86 (98%)	2 (2%)	44	58
23	S	77/87 (88%)	76 (99%)	1 (1%)	61	75
24	T	83/85 (98%)	82 (99%)	1 (1%)	63	76
25	U	79/80 (99%)	77 (98%)	2 (2%)	42	55
26	V	59/64 (92%)	57 (97%)	2 (3%)	32	42
27	W	70/70 (100%)	70 (100%)	0	100	100
28	X	53/56 (95%)	51 (96%)	2 (4%)	29	38
29	Y	53/54 (98%)	52 (98%)	1 (2%)	50	64
30	Z	46/50 (92%)	45 (98%)	1 (2%)	45	59
32	b	185/200 (92%)	178 (96%)	7 (4%)	29	38
33	c	175/198 (88%)	173 (99%)	2 (1%)	65	78
34	d	170/171 (99%)	164 (96%)	6 (4%)	32	41
35	e	113/120 (94%)	111 (98%)	2 (2%)	51	66
36	f	94/111 (85%)	93 (99%)	1 (1%)	65	78
37	g	113/128 (88%)	109 (96%)	4 (4%)	32	41
38	h	108/109 (99%)	107 (99%)	1 (1%)	70	82
39	i	99/100 (99%)	98 (99%)	1 (1%)	68	80
40	j	89/91 (98%)	89 (100%)	0	100	100
41	k	88/98 (90%)	84 (96%)	4 (4%)	24	31
42	l	104/106 (98%)	100 (96%)	4 (4%)	29	38
43	m	95/98 (97%)	92 (97%)	3 (3%)	34	45
44	n	81/82 (99%)	80 (99%)	1 (1%)	63	76
45	o	71/72 (99%)	71 (100%)	0	100	100
46	p	63/77 (82%)	63 (100%)	0	100	100
47	q	71/76 (93%)	68 (96%)	3 (4%)	26	34
48	r	46/66 (70%)	46 (100%)	0	100	100
49	s	70/78 (90%)	68 (97%)	2 (3%)	37	49
50	t	65/67 (97%)	65 (100%)	0	100	100
51	u	53/62 (86%)	52 (98%)	1 (2%)	50	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4483/4756 (94%)	4397 (98%)	86 (2%)	49 64

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	50	ILE
7	C	38	LYS
7	C	272	ARG
7	C	274	LYS
8	D	95	VAL
9	E	5	THR
9	E	6	VAL
9	E	14	SER
9	E	197	VAL
10	F	25	VAL
10	F	51	ASP
10	F	103	LEU
10	F	108	ILE
10	F	112	ARG
10	F	162	THR
11	G	18	THR
11	G	20	ASN
11	G	59	LYS
11	G	127	THR
11	G	165	SER
11	G	170	LEU
13	I	78	THR
15	K	102	VAL
16	L	81	VAL
16	L	135	THR
18	N	36	ILE
18	N	76	LEU
18	N	111	GLU
19	O	28	THR
21	Q	53	VAL
21	Q	87	GLN
21	Q	102	SER
22	R	1	MET
22	R	13	SER
23	S	55	VAL
24	T	24	VAL
25	U	59	VAL

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Mol	Chain	Res	Type
25	U	69	VAL
26	V	10	THR
26	V	80	VAL
28	X	40	SER
28	X	49	THR
29	Y	49	LYS
30	Z	28	THR
32	b	33	ILE
32	b	39	LYS
32	b	42	ILE
32	b	43	ILE
32	b	62	LEU
32	b	82	ILE
32	b	183	ILE
33	c	47	LEU
33	c	139	GLN
34	d	12	SER
34	d	17	THR
34	d	30	VAL
34	d	66	ILE
34	d	175	VAL
34	d	193	LEU
35	e	33	THR
35	e	60	SER
36	f	16	ASP
37	g	6	VAL
37	g	7	VAL
37	g	56	VAL
37	g	73	VAL
38	h	57	LYS
39	i	45	VAL
41	k	29	THR
41	k	67	GLU
41	k	78	LEU
41	k	110	THR
42	l	14	THR
42	l	15	LEU
42	l	59	SER
42	l	115	SER
43	m	63	VAL
43	m	65	THR
43	m	68	ASP

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Mol	Chain	Res	Type
44	n	37	SER
47	q	21	SER
47	q	24	VAL
47	q	30	VAL
49	s	19	VAL
49	s	35	SER
51	u	36	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
4	3	4	GLN
7	C	120	ASN
7	C	163	GLN
8	D	63	ASN
8	D	65	GLN
8	D	133	GLN
8	D	151	GLN
9	E	89	GLN
13	I	12	GLN
13	I	47	HIS
13	I	58	ASN
16	L	22	HIS
18	N	30	ASN
19	O	44	GLN
20	P	101	HIS
21	Q	86	GLN
22	R	62	ASN
24	T	84	GLN
28	X	24	ASN
28	X	61	GLN
30	Z	25	ASN
30	Z	37	HIS
32	b	41	HIS
33	c	3	GLN
33	c	54	ASN
34	d	118	GLN
36	f	58	HIS
36	f	68	GLN
37	g	54	ASN
39	i	48	GLN
40	j	23	GLN

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Mol	Chain	Res	Type
41	k	117	HIS
42	l	96	HIS
45	o	62	GLN
50	t	20	HIS
50	t	80	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
31	a	1527/1544 (98%)	201 (13%)	0
5	A	2722/2918 (93%)	332 (12%)	14 (0%)
6	B	114/115 (99%)	17 (14%)	1 (0%)
All	All	4363/4577 (95%)	550 (12%)	15 (0%)

All (550) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	A	22	G
5	A	53	G
5	A	58	G
5	A	67	G
5	A	68	A
5	A	70	A
5	A	78	A
5	A	81	A
5	A	82	G
5	A	99	A
5	A	104	C
5	A	117	G
5	A	125	A
5	A	126	A
5	A	127	U
5	A	138	A
5	A	147	A
5	A	149	G
5	A	170	A
5	A	203	A
5	A	206	A
5	A	222	G
5	A	223	A
5	A	228	A

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Mol	Chain	Res	Type
5	A	229	A
5	A	235	U
5	A	236	U
5	A	240	A
5	A	255	G
5	A	257	G
5	A	262	A
5	A	272	A
5	A	278	U
5	A	279	U
5	A	297	G
5	A	313	A
5	A	331	G
5	A	332	A
5	A	345	C
5	A	347	A
5	A	348	A
5	A	357	C
5	A	360	A
5	A	365	U
5	A	366	G
5	A	369	G
5	A	370	A
5	A	371	G
5	A	385	G
5	A	395	G
5	A	403	A
5	A	410	G
5	A	416	C
5	A	423	G
5	A	455	C
5	A	480	G
5	A	503	U
5	A	504	A
5	A	508	C
5	A	531	A
5	A	544	U
5	A	546	G
5	A	561	A
5	A	571	U
5	A	573	A
5	A	595	G

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Mol	Chain	Res	Type
5	A	601	A
5	A	611	U
5	A	612	A
5	A	625	A
5	A	626	G
5	A	633	C
5	A	635	A
5	A	643	U
5	A	644	A
5	A	649	G
5	A	651	U
5	A	654	G
5	A	666	A
5	A	684	U
5	A	712	U
5	A	728	A
5	A	745	U
5	A	773	G
5	A	774	G
5	A	780	A
5	A	782	G
5	A	783	G
5	A	803	G
5	A	810	C
5	A	817	A
5	A	825	U
5	A	826	U
5	A	844	A
5	A	845	A
5	A	846	U
5	A	857	G
5	A	864	A
5	A	900	C
5	A	908	A
5	A	929	C
5	A	930	U
5	A	938	A
5	A	942	A
5	A	943	G
5	A	955	U
5	A	958	C
5	A	971	G

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Mol	Chain	Res	Type
5	A	980	A
5	A	981	A
5	A	993	A
5	A	1009	U
5	A	1010	C
5	A	1014	G
5	A	1023	G
5	A	1030	U
5	A	1031	G
5	A	1032	U
5	A	1043	A
5	A	1044	G
5	A	1051	A
5	A	1103	A
5	A	1105	U
5	A	1106	C
5	A	1108	A
5	A	1109	G
5	A	1125	G
5	A	1128	G
5	A	1129	U
5	A	1130	A
5	A	1132	C
5	A	1140	A
5	A	1170	U
5	A	1173	G
5	A	1174	U
5	A	1207	G
5	A	1245	G
5	A	1248	A
5	A	1251	G
5	A	1266	G
5	A	1267	A
5	A	1296	A
5	A	1316	A
5	A	1324	U
5	A	1347	U
5	A	1360	A
5	A	1373	A
5	A	1374	U
5	A	1378	A
5	A	1411	G

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Mol	Chain	Res	Type
5	A	1414	A
5	A	1423	C
5	A	1432	C
5	A	1433	U
5	A	1435	A
5	A	1441	C
5	A	1447	G
5	A	1448	U
5	A	1455	U
5	A	1462	G
5	A	1477	U
5	A	1485	A
5	A	1486	G
5	A	1488	C
5	A	1489	A
5	A	1490	A
5	A	1492	U
5	A	1494	C
5	A	1507	G
5	A	1511	A
5	A	1519	U
5	A	1520	A
5	A	1528	G
5	A	1529	U
5	A	1530	A
5	A	1531	C
5	A	1532	U
5	A	1533	U
5	A	1534	G
5	A	1537	C
5	A	1538	A
5	A	1539	G
5	A	1543	A
5	A	1544	G
5	A	1547	G
5	A	1552	U
5	A	1557	U
5	A	1558	G
5	A	1564	A
5	A	1565	G
5	A	1567	A
5	A	1576	U

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Mol	Chain	Res	Type
5	A	1581	U
5	A	1582	U
5	A	1583	C
5	A	1605	G
5	A	1606	A
5	A	1616	A
5	A	1644	C
5	A	1645	U
5	A	1646	U
5	A	1647	G
5	A	1672	G
5	A	1723	A
5	A	1725	U
5	A	1726	C
5	A	1727	G
5	A	1729	U
5	A	1731	C
5	A	1746	G
5	A	1760	G
5	A	1769	A
5	A	1776	A
5	A	1796	C
5	A	1797	A
5	A	1807	G
5	A	1812	C
5	A	1825	A
5	A	1844	A
5	A	1869	G
5	A	1872	A
5	A	1897	A
5	A	1902	G
5	A	1908	A
5	A	1909	A
5	A	1910	C
5	A	1911	3TD
5	A	1923	A
5	A	1925	G
5	A	1926	G
5	A	1932	A
5	A	1951	U
5	A	1959	U
5	A	1963	C

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Mol	Chain	Res	Type
5	A	1966	A
5	A	1967	U
5	A	1968	G
5	A	1978	U
5	A	1987	U
5	A	1989	U
5	A	2018	U
5	A	2019	C
5	A	2027	A
5	A	2029	A
5	A	2039	C
5	A	2051	C
5	A	2052	G
5	A	2056	A
5	A	2057	G
5	A	2058	A
5	A	2065	7MG
5	A	2089	G
5	A	2194	A
5	A	2200	G
5	A	2207	G
5	A	2221	A
5	A	2234	G
5	A	2235	G
5	A	2264	A
5	A	2279	U
5	A	2283	A
5	A	2299	G
5	A	2301	U
5	A	2303	G
5	A	2304	G
5	A	2305	A
5	A	2306	A
5	A	2318	A
5	A	2321	A
5	A	2323	A
5	A	2341	A
5	A	2343	C
5	A	2346	C
5	A	2378	G
5	A	2379	G
5	A	2380	U

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Mol	Chain	Res	Type
5	A	2381	C
5	A	2398	U
5	A	2402	U
5	A	2421	A
5	A	2425	G
5	A	2426	A
5	A	2430	A
5	A	2431	A
5	A	2437	U
5	A	2444	A
5	A	2469	U
5	A	2470	U
5	A	2471	C
5	A	2472	A
5	A	2498	G
5	A	2499	2MA
5	A	2503	C
5	A	2514	A
5	A	2525	G
5	A	2543	A
5	A	2550	U
5	A	2562	A
5	A	2563	G
5	A	2578	G
5	A	2598	A
5	A	2599	G
5	A	2605	U
5	A	2609	U
5	A	2625	U
5	A	2636	G
5	A	2650	A
5	A	2661	A
5	A	2685	U
5	A	2686	A
5	A	2687	C
5	A	2710	G
5	A	2722	U
5	A	2729	A
5	A	2744	A
5	A	2754	A
5	A	2761	A
5	A	2762	G

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Mol	Chain	Res	Type
5	A	2774	A
5	A	2776	A
5	A	2793	U
5	A	2796	U
5	A	2797	G
5	A	2814	U
5	A	2816	G
5	A	2817	A
5	A	2830	G
5	A	2831	A
5	A	2863	A
5	A	2869	A
5	A	2876	C
5	A	2898	U
6	B	2	C
6	B	22	G
6	B	28	C
6	B	31	G
6	B	32	A
6	B	35	C
6	B	39	C
6	B	40	C
6	B	44	A
6	B	48	A
6	B	54	G
6	B	64	A
6	B	65	G
6	B	71	A
6	B	87	A
6	B	106	A
6	B	115	U
31	a	6	C
31	a	7	U
31	a	9	A
31	a	11	G
31	a	18	A
31	a	24	G
31	a	34	A
31	a	41	G
31	a	49	C
31	a	50	U
31	a	53	A

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Mol	Chain	Res	Type
31	a	62	A
31	a	66	G
31	a	76	A
31	a	77	G
31	a	81	G
31	a	82	C
31	a	83	U
31	a	84	U
31	a	85	G
31	a	91	G
31	a	92	G
31	a	97	A
31	a	117	U
31	a	126	A
31	a	127	U
31	a	159	G
31	a	163	U
31	a	165	C
31	a	170	A
31	a	184	A
31	a	186	G
31	a	193	A
31	a	205	U
31	a	208	G
31	a	216	G
31	a	239	A
31	a	241	U
31	a	243	G
31	a	247	G
31	a	262	G
31	a	263	C
31	a	276	C
31	a	285	G
31	a	324	C
31	a	325	A
31	a	343	G
31	a	348	C
31	a	350	G
31	a	363	U
31	a	368	C
31	a	369	A
31	a	380	C

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Mol	Chain	Res	Type
31	a	402	G
31	a	407	A
31	a	408	A
31	a	409	G
31	a	410	A
31	a	414	C
31	a	418	A
31	a	419	U
31	a	420	G
31	a	425	U
31	a	426	A
31	a	444	A
31	a	447	A
31	a	448	G
31	a	461	A
31	a	463	U
31	a	480	C
31	a	481	G
31	a	483	U
31	a	492	A
31	a	493	A
31	a	496	A
31	a	497	G
31	a	506	A
31	a	508	C
31	a	515	C
31	a	518	G
31	a	524	7MG
31	a	527	G
31	a	528	U
31	a	530	A
31	a	531	U
31	a	544	A
31	a	556	A
31	a	561	C
31	a	569	A
31	a	570	A
31	a	573	C
31	a	574	G
31	a	593	A
31	a	615	C
31	a	630	G

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Mol	Chain	Res	Type
31	a	639	A
31	a	650	A
31	a	662	A
31	a	684	A
31	a	700	G
31	a	720	U
31	a	721	G
31	a	752	G
31	a	774	A
31	a	784	A
31	a	789	A
31	a	790	U
31	a	791	A
31	a	812	A
31	a	814	C
31	a	818	G
31	a	838	U
31	a	839	U
31	a	840	U
31	a	841	G
31	a	846	U
31	a	887	G
31	a	888	U
31	a	911	A
31	a	923	G
31	a	924	G
31	a	931	C
31	a	932	A
31	a	939	G
31	a	957	U
31	a	966	A
31	a	968	G
31	a	972	A
31	a	973	G
31	a	974	A
31	a	989	U
31	a	990	G
31	a	1001	A
31	a	1007	U
31	a	1024	C
31	a	1025	C
31	a	1027	U

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Mol	Chain	Res	Type
31	a	1028	C
31	a	1029	G
31	a	1030	G
31	a	1032	A
31	a	1033	A
31	a	1043	A
31	a	1062	U
31	a	1067	U
31	a	1070	U
31	a	1072	U
31	a	1078	G
31	a	1090	A
31	a	1091	G
31	a	1092	U
31	a	1098	A
31	a	1134	C
31	a	1136	G
31	a	1151	G
31	a	1156	U
31	a	1157	G
31	a	1164	A
31	a	1165	C
31	a	1166	A
31	a	1168	A
31	a	1179	G
31	a	1180	C
31	a	1193	A
31	a	1194	A
31	a	1210	A
31	a	1224	A
31	a	1235	A
31	a	1255	G
31	a	1277	A
31	a	1284	A
31	a	1297	G
31	a	1299	C
31	a	1302	G
31	a	1309	G
31	a	1317	C
31	a	1342	U
31	a	1343	A
31	a	1350	G

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Mol	Chain	Res	Type
31	a	1360	A
31	a	1361	U
31	a	1367	G
31	a	1385	C
31	a	1394	C
31	a	1395	A
31	a	1416	G
31	a	1438	A
31	a	1439	G
31	a	1443	A
31	a	1449	A
31	a	1450	A
31	a	1451	A
31	a	1484	G
31	a	1491	G
31	a	1494	G
31	a	1500	A
31	a	1503	U
31	a	1514	G
31	a	1516	MA6
31	a	1526	G
31	a	1527	G

All (15) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	A	256	C
5	A	364	A
5	A	365	U
5	A	368	C
5	A	424	G
5	A	507	U
5	A	625	A
5	A	782	G
5	A	844	A
5	A	1127	U
5	A	1173	G
5	A	1179	G
5	A	2379	G
5	A	2443	G
6	B	86	U

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

24 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	OMG	A	2247	5	23,26,27	0.48	0	32,38,41	0.45	0
31	MA6	a	1515	31	23,26,27	1.41	4 (17%)	33,38,41	3.22	12 (36%)
5	5MU	A	1935	5	19,22,23	0.45	0	27,32,35	0.49	0
31	MA6	a	1516	31	23,26,27	1.42	4 (17%)	33,38,41	3.25	12 (36%)
5	OMU	A	2548	5	19,22,23	3.03	8 (42%)	25,31,34	1.83	5 (20%)
5	6MZ	A	2026	5	22,25,26	2.51	4 (18%)	29,36,39	3.30	10 (34%)
5	PSU	A	2576	5	18,21,22	1.14	2 (11%)	21,30,33	2.02	6 (28%)
5	PSU	A	2601	5	18,21,22	1.07	1 (5%)	21,30,33	1.93	4 (19%)
31	UR3	a	1495	31	19,22,23	2.88	6 (31%)	26,32,35	1.60	3 (11%)
5	PSU	A	2453	5	18,21,22	1.10	1 (5%)	21,30,33	1.98	6 (28%)
31	4OC	a	1399	31	20,23,24	3.15	8 (40%)	25,32,35	0.89	1 (4%)
5	2MA	A	2499	5	22,25,26	3.92	9 (40%)	32,37,40	2.68	11 (34%)
31	7MG	a	524	31	23,26,27	1.09	1 (4%)	27,39,42	0.87	2 (7%)
5	PSU	A	2500	5	18,21,22	1.10	1 (5%)	21,30,33	1.88	4 (19%)
5	2MG	A	2441	5	23,26,27	0.52	0	33,38,41	0.45	0
5	PSU	A	1907	5	18,21,22	1.15	1 (5%)	21,30,33	1.93	5 (23%)
31	2MG	a	1204	31	23,26,27	0.47	0	33,38,41	0.49	0
5	7MG	A	2065	5	23,26,27	1.03	1 (4%)	27,39,42	0.90	2 (7%)
31	5MC	a	964	31	19,22,23	0.52	0	26,32,35	0.62	0
31	2MG	a	963	31	23,26,27	0.46	0	33,38,41	0.49	0
5	3TD	A	1911	5	19,22,23	4.43	6 (31%)	23,32,35	1.85	4 (17%)
5	PSU	A	952	5	18,21,22	1.10	1 (5%)	21,30,33	1.92	4 (19%)
31	PSU	a	513	31	18,21,22	1.12	1 (5%)	21,30,33	1.91	5 (23%)
5	PSU	A	1913	5	18,21,22	1.10	1 (5%)	21,30,33	1.85	4 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	OMG	A	2247	5	-	1/9/27/28	0/3/3/3
31	MA6	a	1515	31	-	0/11/29/30	0/3/3/3
5	5MU	A	1935	5	-	0/7/25/26	0/2/2/2
31	MA6	a	1516	31	-	0/11/29/30	0/3/3/3
5	OMU	A	2548	5	-	0/9/27/28	0/2/2/2
5	6MZ	A	2026	5	-	2/9/27/28	0/3/3/3
5	PSU	A	2576	5	-	0/7/25/26	0/2/2/2
5	PSU	A	2601	5	-	0/7/25/26	0/2/2/2
31	UR3	a	1495	31	-	0/7/25/26	0/2/2/2
5	PSU	A	2453	5	-	0/7/25/26	0/2/2/2
31	4OC	a	1399	31	-	1/9/29/30	0/2/2/2
5	2MA	A	2499	5	-	2/7/25/26	0/3/3/3
31	7MG	a	524	31	-	2/7/37/38	0/3/3/3
5	PSU	A	2500	5	-	1/7/25/26	0/2/2/2
5	2MG	A	2441	5	-	0/9/27/28	0/3/3/3
5	PSU	A	1907	5	-	0/7/25/26	0/2/2/2
31	2MG	a	1204	31	-	0/9/27/28	0/3/3/3
5	7MG	A	2065	5	-	1/7/37/38	0/3/3/3
31	5MC	a	964	31	-	0/7/25/26	0/2/2/2
31	2MG	a	963	31	-	0/9/27/28	0/3/3/3
5	3TD	A	1911	5	-	2/7/25/26	0/2/2/2
5	PSU	A	952	5	-	0/7/25/26	0/2/2/2
31	PSU	a	513	31	-	0/7/25/26	0/2/2/2
5	PSU	A	1913	5	-	0/7/25/26	0/2/2/2

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1911	3TD	C6-C5	13.30	1.50	1.35
5	A	2499	2MA	C4-N3	11.92	1.49	1.34
5	A	1911	3TD	C2-N1	10.69	1.50	1.37
5	A	2026	6MZ	C6-N6	10.02	1.45	1.34
5	A	2499	2MA	C2-N3	7.25	1.46	1.34
5	A	2548	OMU	C2-N1	7.04	1.49	1.38
31	a	1399	4OC	C4-N3	7.04	1.44	1.32
31	a	1495	UR3	C2-N1	7.02	1.48	1.38
5	A	2499	2MA	C6-N1	6.85	1.44	1.35
31	a	1495	UR3	C6-C5	6.74	1.50	1.35
5	A	2548	OMU	C2-N3	6.71	1.49	1.38
31	a	1399	4OC	C6-C5	6.23	1.49	1.35
31	a	1399	4OC	C2-N3	6.14	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2499	2MA	C2-N1	6.02	1.44	1.34
5	A	1911	3TD	C6-N1	5.72	1.45	1.36
5	A	2548	OMU	C6-C5	5.63	1.48	1.35
31	a	1495	UR3	C2-N3	5.56	1.50	1.39
5	A	1911	3TD	C2-N3	4.94	1.49	1.38
31	a	1399	4OC	C4-N4	4.67	1.45	1.36
5	A	2499	2MA	C5-C6	4.61	1.53	1.41
31	a	524	7MG	C5-N7	4.47	1.41	1.35
5	A	2548	OMU	C4-N3	4.23	1.45	1.38
5	A	2065	7MG	C5-N7	4.20	1.41	1.35
31	a	1399	4OC	C2-N1	4.18	1.48	1.40
31	a	1515	MA6	C6-N6	3.90	1.47	1.36
31	a	1516	MA6	C6-N6	3.87	1.47	1.36
5	A	1907	PSU	C6-C5	3.79	1.39	1.35
5	A	1913	PSU	C6-C5	3.71	1.39	1.35
5	A	2500	PSU	C6-C5	3.62	1.39	1.35
31	a	513	PSU	C6-C5	3.60	1.39	1.35
31	a	1399	4OC	C5-C4	3.56	1.48	1.41
5	A	2576	PSU	C6-C5	3.53	1.39	1.35
5	A	2499	2MA	C6-N6	-3.51	1.25	1.34
5	A	952	PSU	C6-C5	3.49	1.39	1.35
5	A	2453	PSU	C6-C5	3.41	1.39	1.35
5	A	2601	PSU	C6-C5	3.41	1.39	1.35
31	a	1495	UR3	C6-N1	3.32	1.46	1.38
31	a	1399	4OC	C6-N1	3.30	1.46	1.38
5	A	2026	6MZ	C5-N7	-3.20	1.33	1.39
5	A	1911	3TD	C4-N3	3.05	1.46	1.40
31	a	1516	MA6	C5-C4	-3.03	1.33	1.39
5	A	2548	OMU	O4-C4	-3.02	1.18	1.24
31	a	1515	MA6	C5-C4	-3.02	1.33	1.39
5	A	2026	6MZ	C5-C4	-3.01	1.33	1.39
31	a	1399	4OC	O2-C2	-2.83	1.18	1.23
5	A	2548	OMU	C6-N1	2.79	1.44	1.38
31	a	1495	UR3	C4-N3	2.58	1.45	1.40
5	A	2548	OMU	O2-C2	-2.56	1.18	1.23
5	A	2499	2MA	C5-N7	-2.56	1.34	1.39
5	A	2026	6MZ	C8-N9	-2.56	1.33	1.37
31	a	1516	MA6	C5-N7	-2.46	1.34	1.39
5	A	2499	2MA	C4-N9	-2.44	1.32	1.37
31	a	1515	MA6	C5-N7	-2.40	1.34	1.39
5	A	2548	OMU	C5-C4	2.35	1.48	1.43
5	A	1911	3TD	O2-C2	-2.32	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	1516	MA6	C8-N9	-2.31	1.33	1.37
31	a	1495	UR3	C5-C4	2.27	1.49	1.43
31	a	1515	MA6	C8-N9	-2.25	1.33	1.37
5	A	2499	2MA	C8-N7	2.15	1.35	1.31
5	A	2576	PSU	O4'-C1'	-2.10	1.40	1.43

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	1516	MA6	N1-C6-N6	-11.77	102.51	116.86
31	a	1515	MA6	N1-C6-N6	-11.73	102.57	116.86
5	A	2026	6MZ	C4-N9-C1'	-8.94	105.73	126.63
5	A	2026	6MZ	C1'-N9-C8	8.82	146.66	127.09
31	a	1516	MA6	C5-C6-N6	7.84	137.74	125.33
31	a	1515	MA6	C5-C6-N6	7.78	137.64	125.33
5	A	2499	2MA	C1'-N9-C8	-7.07	111.40	127.09
5	A	2499	2MA	N9-C8-N7	-5.95	105.49	113.94
5	A	2026	6MZ	C5-C4-N3	-5.91	118.58	126.72
5	A	1911	3TD	N1-C2-N3	5.80	120.35	116.13
5	A	2548	OMU	C4-N3-C2	-5.72	119.51	126.61
31	a	1515	MA6	N1-C2-N3	-5.67	120.00	128.58
31	a	1495	UR3	C4-N3-C2	-5.64	120.04	124.58
31	a	1516	MA6	N1-C2-N3	-5.57	120.16	128.58
5	A	2499	2MA	C5-C4-N3	-5.37	121.52	127.18
5	A	2499	2MA	C4-N9-C8	5.15	111.15	105.74
5	A	2026	6MZ	N1-C2-N3	-5.13	120.81	128.58
5	A	2026	6MZ	C4-C5-C6	5.03	120.96	116.78
5	A	2453	PSU	C4-N3-C2	-4.97	119.52	126.37
5	A	2576	PSU	N1-C2-N3	4.95	120.39	115.17
5	A	2453	PSU	N1-C2-N3	4.94	120.38	115.17
5	A	2601	PSU	C4-N3-C2	-4.92	119.59	126.37
5	A	952	PSU	N1-C2-N3	4.87	120.30	115.17
5	A	2601	PSU	N1-C2-N3	4.86	120.29	115.17
5	A	952	PSU	C4-N3-C2	-4.82	119.73	126.37
5	A	1907	PSU	C4-N3-C2	-4.79	119.77	126.37
31	a	1516	MA6	C5-C4-N3	-4.79	120.12	126.72
5	A	2500	PSU	C4-N3-C2	-4.77	119.81	126.37
5	A	1907	PSU	N1-C2-N3	4.76	120.19	115.17
31	a	513	PSU	N1-C2-N3	4.75	120.18	115.17
5	A	2500	PSU	N1-C2-N3	4.75	120.18	115.17
5	A	2576	PSU	C4-N3-C2	-4.72	119.87	126.37
5	A	1913	PSU	N1-C2-N3	4.69	120.11	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	513	PSU	C4-N3-C2	-4.67	119.93	126.37
5	A	1913	PSU	C4-N3-C2	-4.64	119.97	126.37
31	a	1515	MA6	C5-C4-N3	-4.64	120.33	126.72
5	A	2499	2MA	C4-N9-C1'	4.63	137.45	126.63
31	a	1515	MA6	N9-C8-N7	-4.37	107.74	113.94
31	a	1516	MA6	N9-C8-N7	-4.36	107.76	113.94
5	A	1911	3TD	C4-N3-C2	-4.31	120.05	124.61
5	A	2026	6MZ	N3-C4-N9	4.08	134.11	127.17
31	a	1516	MA6	C4-C5-C6	4.02	120.07	115.91
5	A	2499	2MA	N3-C4-N9	3.97	132.03	126.99
5	A	2548	OMU	N3-C2-N1	3.94	120.03	114.89
31	a	1515	MA6	C4-C5-C6	3.80	119.84	115.91
31	a	1495	UR3	C5-C4-N3	3.72	119.93	115.04
5	A	2548	OMU	C5-C4-N3	3.66	119.93	114.80
5	A	2026	6MZ	N9-C8-N7	-3.65	108.76	113.94
5	A	2026	6MZ	C2-N3-C4	3.47	120.30	111.83
31	a	1515	MA6	C2-N1-C6	3.45	120.26	111.83
5	A	2499	2MA	N3-C2-N1	-3.39	119.79	125.77
5	A	2499	2MA	C5-N7-C8	3.38	108.76	103.45
31	a	1516	MA6	C2-N1-C6	3.38	120.08	111.83
31	a	1516	MA6	C2-N3-C4	3.27	119.81	111.83
31	a	1515	MA6	C2-N3-C4	3.26	119.79	111.83
5	A	2576	PSU	O2-C2-N1	-3.04	119.65	122.79
31	a	1516	MA6	N3-C4-N9	2.99	132.25	127.17
5	A	2500	PSU	O2-C2-N1	-2.96	119.74	122.79
31	a	1515	MA6	N3-C4-N9	2.93	132.15	127.17
5	A	2548	OMU	O4-C4-C5	-2.92	120.12	125.16
31	a	1516	MA6	C5-N7-C8	2.88	107.98	103.45
31	a	1515	MA6	C5-N7-C8	2.85	107.93	103.45
5	A	1907	PSU	O2-C2-N1	-2.76	119.94	122.79
5	A	2576	PSU	C6-N1-C2	-2.75	120.14	122.69
5	A	2026	6MZ	C5-N7-C8	2.74	107.75	103.45
31	a	1515	MA6	C4-N9-C8	2.68	108.55	105.74
31	a	513	PSU	O2-C2-N1	-2.67	120.03	122.79
31	a	1516	MA6	C4-N9-C8	2.62	108.49	105.74
5	A	952	PSU	O2-C2-N1	-2.61	120.09	122.79
5	A	2576	PSU	O4'-C1'-C2'	2.57	108.70	105.15
5	A	1913	PSU	O2-C2-N1	-2.55	120.16	122.79
5	A	2453	PSU	O2-C2-N1	-2.55	120.16	122.79
5	A	1911	3TD	C6-C5-C4	2.53	119.89	118.19
31	a	513	PSU	C6-N1-C2	-2.52	120.35	122.69
5	A	1913	PSU	C6-N1-C2	-2.50	120.38	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2065	7MG	C4-C5-N7	2.50	108.32	105.38
31	a	524	7MG	C4-C5-N7	2.48	108.31	105.38
5	A	1907	PSU	C6-N1-C2	-2.40	120.47	122.69
5	A	2453	PSU	C6-N1-C2	-2.39	120.48	122.69
5	A	952	PSU	C6-N1-C2	-2.38	120.48	122.69
5	A	2500	PSU	C6-N1-C2	-2.38	120.48	122.69
5	A	2499	2MA	CM2-C2-N1	2.38	120.68	117.13
31	a	513	PSU	O4'-C1'-C2'	2.34	108.39	105.15
5	A	2026	6MZ	C5-C6-N1	2.33	120.66	118.15
5	A	2601	PSU	C6-N1-C2	-2.31	120.55	122.69
5	A	2601	PSU	O2-C2-N1	-2.30	120.42	122.79
5	A	2548	OMU	O2-C2-N1	-2.23	119.89	122.80
5	A	1907	PSU	C6-C5-C4	2.23	119.68	118.17
31	a	1399	4OC	C6-C5-C4	2.22	119.68	117.00
5	A	2499	2MA	N6-C6-N1	2.20	120.00	117.03
31	a	524	7MG	C5-C4-N9	2.20	109.15	106.33
5	A	2065	7MG	C5-C4-N9	2.19	109.14	106.33
5	A	2453	PSU	C6-C5-C4	2.15	119.62	118.17
5	A	2576	PSU	C6-C5-C4	2.13	119.61	118.17
31	a	1516	MA6	C4-C5-N7	-2.13	108.15	110.58
5	A	2499	2MA	C4-C5-N7	-2.12	108.16	110.58
5	A	2453	PSU	O4'-C1'-C2'	2.08	108.03	105.15
5	A	1911	3TD	C1'-C5-C4	2.07	120.75	117.61
31	a	1495	UR3	C6-N1-C2	-2.06	120.11	121.80
31	a	1515	MA6	C4-C5-N7	-2.04	108.25	110.58

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1911	3TD	C3'-C4'-C5'-O5'
5	A	1911	3TD	O4'-C4'-C5'-O5'
5	A	2247	OMG	C1'-C2'-O2'-CM2
5	A	2499	2MA	O4'-C4'-C5'-O5'
31	a	524	7MG	C3'-C4'-C5'-O5'
5	A	2499	2MA	C3'-C4'-C5'-O5'
5	A	2026	6MZ	O4'-C4'-C5'-O5'
5	A	2026	6MZ	C3'-C4'-C5'-O5'
31	a	524	7MG	O4'-C4'-C5'-O5'
31	a	1399	4OC	O4'-C4'-C5'-O5'
5	A	2500	PSU	O4'-C4'-C5'-O5'
5	A	2065	7MG	C4'-C5'-O5'-P

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2247	OMG	1	0
5	A	1935	5MU	1	0
5	A	2026	6MZ	2	0
31	a	1399	4OC	1	0
31	a	964	5MC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
53	OIY	a	1604	-	36,37,55	1.35	6 (16%)	37,52,74	1.65	5 (13%)
53	OIY	A	3004	-	54,55,55	1.78	11 (20%)	55,74,74	1.55	7 (12%)
53	OIY	a	1601	-	36,37,55	1.35	6 (16%)	37,52,74	1.74	5 (13%)
53	OIY	A	3005	-	54,55,55	1.79	10 (18%)	55,74,74	1.54	7 (12%)
53	OIY	a	1603	-	54,55,55	1.79	11 (20%)	55,74,74	1.57	7 (12%)
53	OIY	A	3007	-	41,42,55	1.67	9 (21%)	43,58,74	1.64	6 (13%)
53	OIY	A	3001	-	36,37,55	1.36	6 (16%)	37,52,74	1.72	5 (13%)
53	OIY	A	3003	-	32,33,55	1.44	6 (18%)	34,47,74	1.73	5 (14%)
53	OIY	a	1602	-	54,55,55	1.79	11 (20%)	55,74,74	1.49	8 (14%)
53	OIY	W	101	-	54,55,55	1.80	11 (20%)	55,74,74	1.52	6 (10%)
53	OIY	A	3006	-	41,42,55	1.72	9 (21%)	43,58,74	1.65	6 (13%)
53	OIY	A	3002	-	36,37,55	1.35	6 (16%)	37,52,74	2.00	7 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	OIY	a	1604	-	-	3/22/67/89	0/3/3/3
53	OIY	A	3004	-	-	11/44/89/89	0/3/3/3
53	OIY	a	1601	-	-	4/22/67/89	0/3/3/3
53	OIY	A	3005	-	-	17/44/89/89	0/3/3/3
53	OIY	a	1603	-	-	13/44/89/89	0/3/3/3
53	OIY	A	3007	-	-	5/28/73/89	0/3/3/3
53	OIY	A	3001	-	-	8/22/67/89	0/3/3/3
53	OIY	A	3003	-	-	5/17/62/89	0/3/3/3
53	OIY	a	1602	-	-	13/44/89/89	0/3/3/3
53	OIY	W	101	-	-	9/44/89/89	0/3/3/3
53	OIY	A	3006	-	-	9/28/73/89	0/3/3/3
53	OIY	A	3002	-	-	7/22/67/89	0/3/3/3

All (102) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	A	3006	OIY	C34-N33	6.81	1.49	1.33
53	a	1602	OIY	C34-N33	6.74	1.49	1.33
53	A	3005	OIY	C34-N33	6.71	1.49	1.33
53	a	1603	OIY	C34-N33	6.70	1.49	1.33
53	W	101	OIY	C34-N33	6.69	1.49	1.33
53	A	3007	OIY	C34-N33	6.66	1.49	1.33
53	A	3004	OIY	C34-N33	6.65	1.49	1.33
53	A	3005	OIY	C42-N41	6.14	1.48	1.33
53	W	101	OIY	C42-N41	6.14	1.47	1.33
53	a	1602	OIY	C42-N41	6.11	1.47	1.33
53	A	3004	OIY	C42-N41	6.08	1.47	1.33
53	a	1603	OIY	C42-N41	6.07	1.47	1.33
53	a	1603	OIY	C05-N07	3.93	1.40	1.33
53	W	101	OIY	C05-N07	3.91	1.40	1.33
53	A	3001	OIY	C05-N07	3.88	1.40	1.33
53	a	1602	OIY	C05-N07	3.87	1.40	1.33
53	A	3003	OIY	C05-N07	3.87	1.40	1.33
53	A	3004	OIY	C05-N07	3.83	1.40	1.33
53	a	1604	OIY	C05-N07	3.82	1.40	1.33
53	A	3005	OIY	C05-N07	3.79	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	a	1601	OIY	C05-N07	3.77	1.40	1.33
53	A	3006	OIY	C05-N07	3.74	1.40	1.33
53	A	3002	OIY	C05-N07	3.70	1.40	1.33
53	A	3007	OIY	C05-N07	3.67	1.40	1.33
53	A	3002	OIY	C01-C02	3.25	1.55	1.52
53	A	3004	OIY	C01-C02	3.25	1.55	1.52
53	W	101	OIY	C01-C02	3.24	1.55	1.52
53	A	3003	OIY	C01-C02	3.23	1.55	1.52
53	A	3006	OIY	C01-C02	3.21	1.55	1.52
53	a	1604	OIY	C01-C02	3.19	1.55	1.52
53	A	3005	OIY	C01-C02	3.19	1.55	1.52
53	a	1601	OIY	C01-C02	3.18	1.55	1.52
53	A	3007	OIY	C01-C02	3.18	1.55	1.52
53	A	3001	OIY	C01-C02	3.16	1.55	1.52
53	a	1603	OIY	C01-C02	3.09	1.55	1.52
53	a	1602	OIY	C01-C02	3.05	1.55	1.52
53	a	1602	OIY	C02-C03	-2.90	1.50	1.53
53	A	3001	OIY	C02-C03	-2.88	1.50	1.53
53	A	3005	OIY	C02-C03	-2.85	1.50	1.53
53	a	1604	OIY	C02-C03	-2.85	1.50	1.53
53	a	1603	OIY	C02-C03	-2.85	1.50	1.53
53	A	3004	OIY	C02-C03	-2.84	1.50	1.53
53	W	101	OIY	C02-C03	-2.81	1.50	1.53
53	A	3006	OIY	C02-C03	-2.81	1.50	1.53
53	A	3003	OIY	C02-C03	-2.80	1.50	1.53
53	a	1601	OIY	C02-C03	-2.77	1.50	1.53
53	W	101	OIY	C01-N07	2.76	1.49	1.46
53	A	3002	OIY	C02-C03	-2.72	1.50	1.53
53	A	3007	OIY	C02-C03	-2.71	1.50	1.53
53	a	1603	OIY	C01-N07	2.70	1.49	1.46
53	a	1601	OIY	C01-N07	2.69	1.49	1.46
53	a	1604	OIY	C01-N07	2.68	1.49	1.46
53	A	3003	OIY	C01-N07	2.66	1.49	1.46
53	A	3002	OIY	C01-N07	2.66	1.49	1.46
53	A	3001	OIY	C01-N07	2.65	1.49	1.46
53	A	3005	OIY	C01-N07	2.64	1.49	1.46
53	a	1602	OIY	C01-N07	2.61	1.49	1.46
53	A	3004	OIY	C01-N07	2.58	1.49	1.46
53	A	3006	OIY	C01-N07	2.55	1.49	1.46
53	A	3002	OIY	C26-N25	2.50	1.39	1.34
53	A	3004	OIY	C26-N25	2.44	1.39	1.34
53	W	101	OIY	C26-N25	2.41	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	A	3003	OIY	C26-N25	2.41	1.39	1.34
53	A	3006	OIY	C36-C34	2.41	1.56	1.51
53	a	1603	OIY	C26-N25	2.40	1.39	1.34
53	a	1601	OIY	C26-N25	2.38	1.39	1.34
53	a	1604	OIY	C26-N25	2.38	1.39	1.34
53	A	3005	OIY	C26-N25	2.37	1.39	1.34
53	A	3006	OIY	C26-N25	2.37	1.39	1.34
53	a	1602	OIY	C26-N25	2.36	1.39	1.34
53	A	3001	OIY	C26-N25	2.35	1.39	1.34
53	A	3007	OIY	C36-C34	2.34	1.56	1.51
53	A	3007	OIY	C26-N25	2.32	1.38	1.34
53	A	3005	OIY	C21-N23	2.32	1.37	1.33
53	a	1602	OIY	C21-N23	2.30	1.37	1.33
53	W	101	OIY	C21-N23	2.30	1.37	1.33
53	a	1603	OIY	C21-N23	2.29	1.37	1.33
53	A	3007	OIY	C21-N23	2.29	1.37	1.33
53	A	3004	OIY	C21-N23	2.28	1.37	1.33
53	a	1601	OIY	C21-N23	2.28	1.37	1.33
53	A	3006	OIY	C21-N23	2.27	1.37	1.33
53	A	3001	OIY	C21-N23	2.26	1.37	1.33
53	A	3007	OIY	C01-N07	2.26	1.48	1.46
53	A	3002	OIY	C21-N23	2.24	1.37	1.33
53	A	3003	OIY	C21-N23	2.24	1.37	1.33
53	a	1604	OIY	C21-N23	2.21	1.37	1.33
53	A	3005	OIY	O43-C42	-2.15	1.19	1.23
53	a	1602	OIY	O43-C42	-2.13	1.19	1.23
53	A	3004	OIY	O43-C42	-2.12	1.19	1.23
53	A	3005	OIY	O35-C34	-2.11	1.19	1.23
53	a	1603	OIY	O43-C42	-2.10	1.19	1.23
53	W	101	OIY	O43-C42	-2.10	1.19	1.23
53	a	1603	OIY	O35-C34	-2.10	1.19	1.23
53	A	3004	OIY	O35-C34	-2.09	1.19	1.23
53	a	1602	OIY	O35-C34	-2.09	1.19	1.23
53	A	3007	OIY	O35-C34	-2.06	1.19	1.23
53	W	101	OIY	C36-C34	2.06	1.56	1.51
53	A	3006	OIY	O35-C34	-2.06	1.19	1.23
53	W	101	OIY	O35-C34	-2.05	1.19	1.23
53	a	1603	OIY	C36-C34	2.02	1.56	1.51
53	A	3004	OIY	C36-C34	2.01	1.56	1.51
53	a	1602	OIY	C36-C34	2.00	1.56	1.51

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	A	3006	OIY	C02-C01-N07	7.62	117.59	109.83
53	A	3007	OIY	C02-C01-N07	7.47	117.44	109.83
53	a	1601	OIY	C02-C01-N07	7.43	117.40	109.83
53	A	3004	OIY	C02-C01-N07	7.35	117.31	109.83
53	A	3002	OIY	C02-C01-N07	7.34	117.30	109.83
53	W	101	OIY	C02-C01-N07	7.25	117.22	109.83
53	A	3001	OIY	C02-C01-N07	7.24	117.21	109.83
53	A	3003	OIY	C02-C01-N07	7.23	117.20	109.83
53	a	1603	OIY	C02-C01-N07	7.21	117.18	109.83
53	a	1604	OIY	C02-C01-N07	7.20	117.16	109.83
53	A	3005	OIY	C02-C01-N07	7.10	117.06	109.83
53	a	1602	OIY	C02-C01-N07	7.04	117.00	109.83
53	A	3002	OIY	C12-C13-N25	4.91	117.11	111.12
53	A	3002	OIY	C13-N25-C26	3.72	128.38	122.90
53	A	3003	OIY	O17-C12-C13	3.70	111.50	108.97
53	a	1601	OIY	O06-C05-N07	3.63	127.33	122.41
53	A	3002	OIY	O06-C05-N07	3.59	127.28	122.41
53	A	3002	OIY	C28-C26-N25	-3.53	111.44	116.25
53	W	101	OIY	C28-C26-N25	-3.48	111.51	116.25
53	a	1603	OIY	C36-C34-N33	3.47	121.33	115.97
53	A	3004	OIY	C28-C26-N25	-3.42	111.59	116.25
53	A	3001	OIY	O06-C05-N07	3.40	127.02	122.41
53	A	3001	OIY	C28-C26-N25	-3.38	111.64	116.25
53	a	1603	OIY	C28-C26-N25	-3.38	111.64	116.25
53	a	1602	OIY	C28-C26-N25	-3.37	111.65	116.25
53	a	1604	OIY	O06-C05-N07	3.36	126.96	122.41
53	A	3005	OIY	C28-C26-N25	-3.33	111.71	116.25
53	a	1601	OIY	C28-C26-N25	-3.29	111.76	116.25
53	A	3001	OIY	O17-C12-C13	3.27	111.20	108.97
53	a	1604	OIY	C28-C26-N25	-3.26	111.81	116.25
53	A	3006	OIY	C28-C26-N25	-3.25	111.81	116.25
53	a	1603	OIY	O06-C05-N07	3.24	126.81	122.41
53	A	3003	OIY	O06-C05-N07	3.24	126.80	122.41
53	W	101	OIY	O06-C05-N07	3.24	126.80	122.41
53	a	1601	OIY	O17-C12-C13	3.20	111.15	108.97
53	A	3004	OIY	O06-C05-N07	3.19	126.73	122.41
53	A	3007	OIY	C28-C26-N25	-3.16	111.94	116.25
53	A	3005	OIY	O06-C05-N07	3.11	126.63	122.41
53	A	3006	OIY	C36-C34-N33	3.06	121.91	116.34
53	a	1602	OIY	C03-N10-C09	-3.04	107.09	112.17
53	A	3004	OIY	C36-C34-N33	3.03	120.66	115.97
53	W	101	OIY	C03-N10-C09	-2.96	107.22	112.17
53	A	3005	OIY	C44-C42-N41	2.96	120.54	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	A	3006	OIY	O06-C05-N07	2.88	126.31	122.41
53	a	1601	OIY	C03-N10-C09	-2.84	107.42	112.17
53	a	1604	OIY	C03-N10-C09	-2.83	107.43	112.17
53	a	1603	OIY	C03-N10-C09	-2.81	107.47	112.17
53	a	1602	OIY	O06-C05-N07	2.80	126.20	122.41
53	A	3001	OIY	C03-N10-C09	-2.80	107.50	112.17
53	A	3005	OIY	C03-N10-C09	-2.76	107.56	112.17
53	A	3002	OIY	C03-N10-C09	-2.75	107.58	112.17
53	A	3003	OIY	C03-N10-C09	-2.69	107.68	112.17
53	A	3004	OIY	C03-N10-C09	-2.66	107.72	112.17
53	W	101	OIY	C44-C42-N41	2.55	119.91	115.97
53	A	3004	OIY	C44-C42-N41	2.52	119.87	115.97
53	A	3006	OIY	C03-N10-C09	-2.47	108.04	112.17
53	a	1603	OIY	O17-C12-C13	2.46	110.64	108.97
53	A	3003	OIY	C28-C26-N25	-2.41	111.62	115.86
53	W	101	OIY	C36-C34-N33	2.40	119.68	115.97
53	a	1603	OIY	C44-C42-N41	2.37	119.64	115.97
53	A	3007	OIY	O06-C05-N07	2.33	125.57	122.41
53	a	1602	OIY	C40-N41-C42	-2.28	118.58	122.82
53	A	3005	OIY	C40-N41-C42	-2.26	118.61	122.82
53	A	3005	OIY	C36-C34-N33	2.26	119.46	115.97
53	A	3007	OIY	O17-C12-N11	2.25	112.24	108.12
53	a	1604	OIY	O17-C12-C13	2.23	110.49	108.97
53	A	3007	OIY	C36-C34-N33	2.22	120.38	116.34
53	a	1602	OIY	C36-C34-N33	2.21	119.39	115.97
53	a	1602	OIY	O17-C12-N11	2.14	112.04	108.12
53	a	1602	OIY	C44-C42-N41	2.12	119.25	115.97
53	A	3007	OIY	C03-N10-C09	-2.04	108.76	112.17
53	A	3002	OIY	O27-C26-N25	2.02	126.37	122.95
53	A	3004	OIY	C32-N33-C34	-2.01	119.08	122.82
53	A	3006	OIY	O35-C34-N33	-2.01	119.09	123.03

There are no chirality outliers.

All (104) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
53	A	3001	OIY	C26-C28-C29-C30
53	A	3001	OIY	C26-C28-C29-N52
53	A	3001	OIY	C28-C29-C30-C31
53	A	3002	OIY	C12-C13-N25-C26
53	A	3002	OIY	C14-C15-O20-C21
53	A	3002	OIY	C16-C15-O20-C21

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Mol	Chain	Res	Type	Atoms
53	A	3002	OIY	C26-C28-C29-C30
53	A	3002	OIY	C26-C28-C29-N52
53	A	3003	OIY	N23-C21-O20-C15
53	A	3003	OIY	O22-C21-O20-C15
53	A	3004	OIY	C26-C28-C29-N52
53	A	3004	OIY	C36-C37-C38-C39
53	A	3005	OIY	O17-C12-N11-C09
53	A	3005	OIY	C28-C29-C30-C31
53	A	3005	OIY	C29-C30-C31-C32
53	A	3005	OIY	C34-C36-C37-C38
53	A	3005	OIY	C34-C36-C37-N51
53	A	3005	OIY	N51-C37-C38-C39
53	A	3005	OIY	N50-C45-C46-C47
53	W	101	OIY	N23-C21-O20-C15
53	W	101	OIY	O22-C21-O20-C15
53	a	1601	OIY	C26-C28-C29-C30
53	a	1601	OIY	C26-C28-C29-N52
53	a	1602	OIY	C26-C28-C29-N52
53	a	1602	OIY	C34-C36-C37-C38
53	a	1602	OIY	C34-C36-C37-N51
53	a	1603	OIY	C34-C36-C37-N51
53	A	3001	OIY	O17-C16-C18-O19
53	A	3006	OIY	C36-C34-N33-C32
53	W	101	OIY	C44-C42-N41-C40
53	a	1602	OIY	C44-C42-N41-C40
53	a	1603	OIY	C36-C34-N33-C32
53	A	3005	OIY	O17-C16-C18-O19
53	W	101	OIY	O17-C16-C18-O19
53	A	3003	OIY	O17-C16-C18-O19
53	A	3001	OIY	C15-C16-C18-O19
53	A	3004	OIY	C15-C16-C18-O19
53	A	3007	OIY	C15-C16-C18-O19
53	A	3003	OIY	C15-C16-C18-O19
53	A	3007	OIY	C30-C31-C32-N33
53	A	3007	OIY	O17-C16-C18-O19
53	A	3006	OIY	O35-C34-N33-C32
53	W	101	OIY	O43-C42-N41-C40
53	a	1602	OIY	O43-C42-N41-C40
53	a	1603	OIY	O35-C34-N33-C32
53	A	3004	OIY	C30-C31-C32-N33
53	W	101	OIY	C38-C39-C40-N41
53	A	3005	OIY	C15-C16-C18-O19

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Mol	Chain	Res	Type	Atoms
53	A	3004	OIY	O17-C16-C18-O19
53	W	101	OIY	C15-C16-C18-O19
53	a	1604	OIY	O17-C16-C18-O19
53	W	101	OIY	C26-C28-C29-C30
53	a	1603	OIY	C42-C44-C45-C46
53	a	1602	OIY	O17-C16-C18-O19
53	a	1603	OIY	C15-C16-C18-O19
53	a	1603	OIY	O17-C16-C18-O19
53	A	3006	OIY	N25-C26-C28-C29
53	A	3006	OIY	C26-C28-C29-C30
53	a	1603	OIY	C38-C39-C40-N41
53	A	3006	OIY	O27-C26-C28-C29
53	a	1602	OIY	C38-C39-C40-N41
53	a	1602	OIY	N23-C21-O20-C15
53	a	1602	OIY	O22-C21-O20-C15
53	W	101	OIY	C34-C36-C37-N51
53	A	3001	OIY	C14-C15-O20-C21
53	a	1602	OIY	C14-C15-O20-C21
53	a	1603	OIY	C14-C15-O20-C21
53	A	3005	OIY	C36-C37-C38-C39
53	a	1603	OIY	C28-C29-C30-C31
53	a	1603	OIY	N52-C29-C30-C31
53	A	3004	OIY	C26-C28-C29-C30
53	a	1603	OIY	C34-C36-C37-C38
53	A	3004	OIY	C37-C38-C39-C40
53	a	1603	OIY	C30-C31-C32-N33
53	a	1601	OIY	C30-C31-C32-N33
53	A	3006	OIY	C34-C36-C37-N51
53	a	1604	OIY	C15-C16-C18-O19
53	A	3005	OIY	O35-C34-C36-C37
53	A	3005	OIY	N33-C34-C36-C37
53	A	3006	OIY	C31-C32-N33-C34
53	A	3006	OIY	O35-C34-C36-C37
53	a	1602	OIY	C29-C30-C31-C32
53	A	3004	OIY	C38-C39-C40-N41
53	A	3005	OIY	C42-C44-C45-N50
53	A	3007	OIY	C26-C28-C29-N52
53	a	1603	OIY	C42-C44-C45-N50
53	A	3005	OIY	N41-C42-C44-C45
53	A	3004	OIY	C29-C30-C31-C32
53	A	3002	OIY	O27-C26-C28-C29
53	A	3004	OIY	O35-C34-C36-C37

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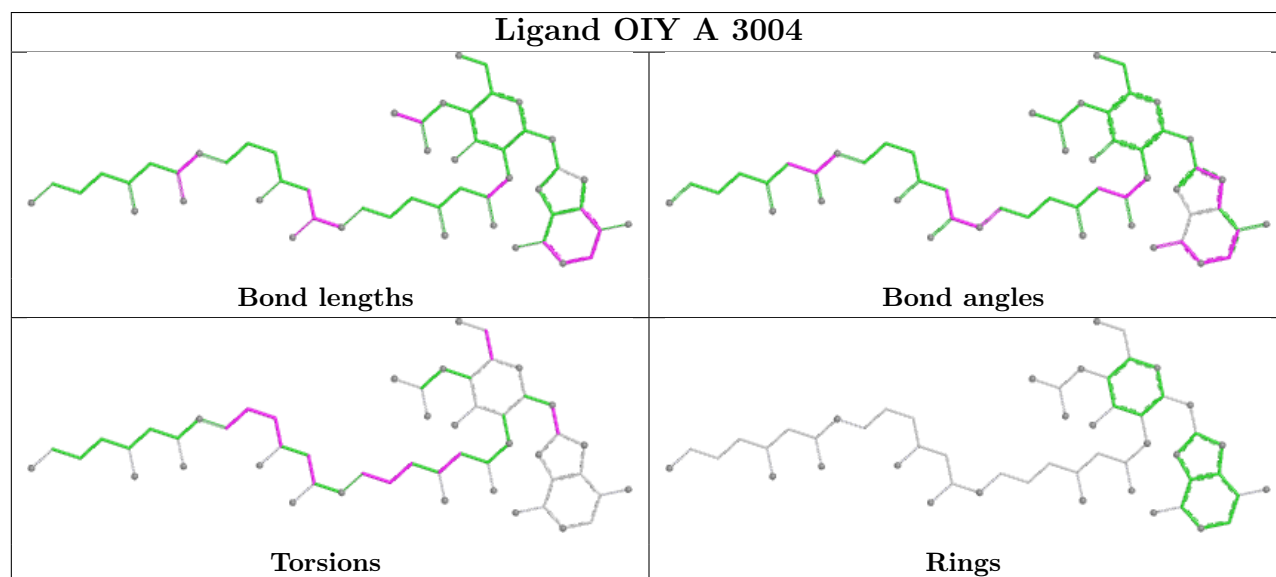
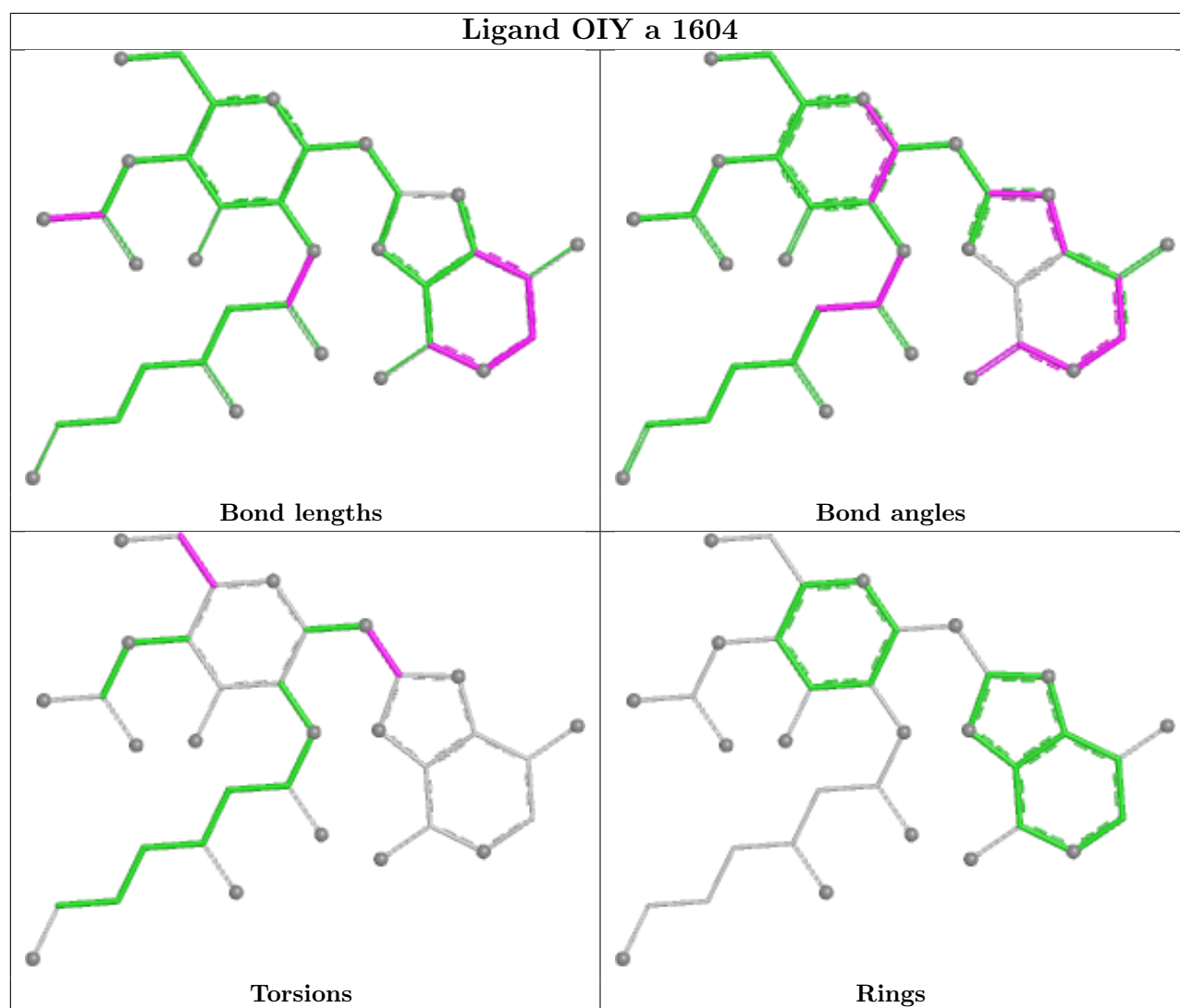
Mol	Chain	Res	Type	Atoms
53	A	3005	OIY	O43-C42-C44-C45
53	a	1602	OIY	O27-C26-C28-C29
53	A	3001	OIY	N52-C29-C30-C31
53	A	3001	OIY	N08-C09-N11-C12
53	A	3002	OIY	N08-C09-N11-C12
53	A	3003	OIY	N08-C09-N11-C12
53	A	3004	OIY	N08-C09-N11-C12
53	A	3005	OIY	N52-C29-C30-C31
53	A	3005	OIY	N08-C09-N11-C12
53	A	3006	OIY	N08-C09-N11-C12
53	A	3007	OIY	N08-C09-N11-C12
53	a	1601	OIY	N08-C09-N11-C12
53	a	1604	OIY	N08-C09-N11-C12
53	a	1602	OIY	N25-C26-C28-C29

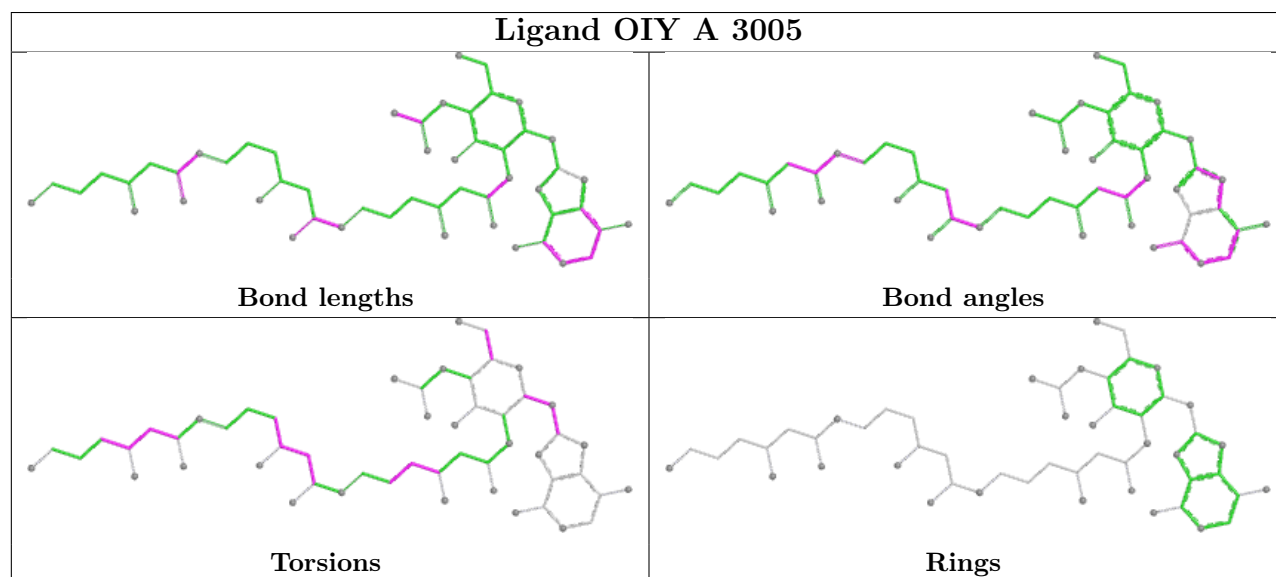
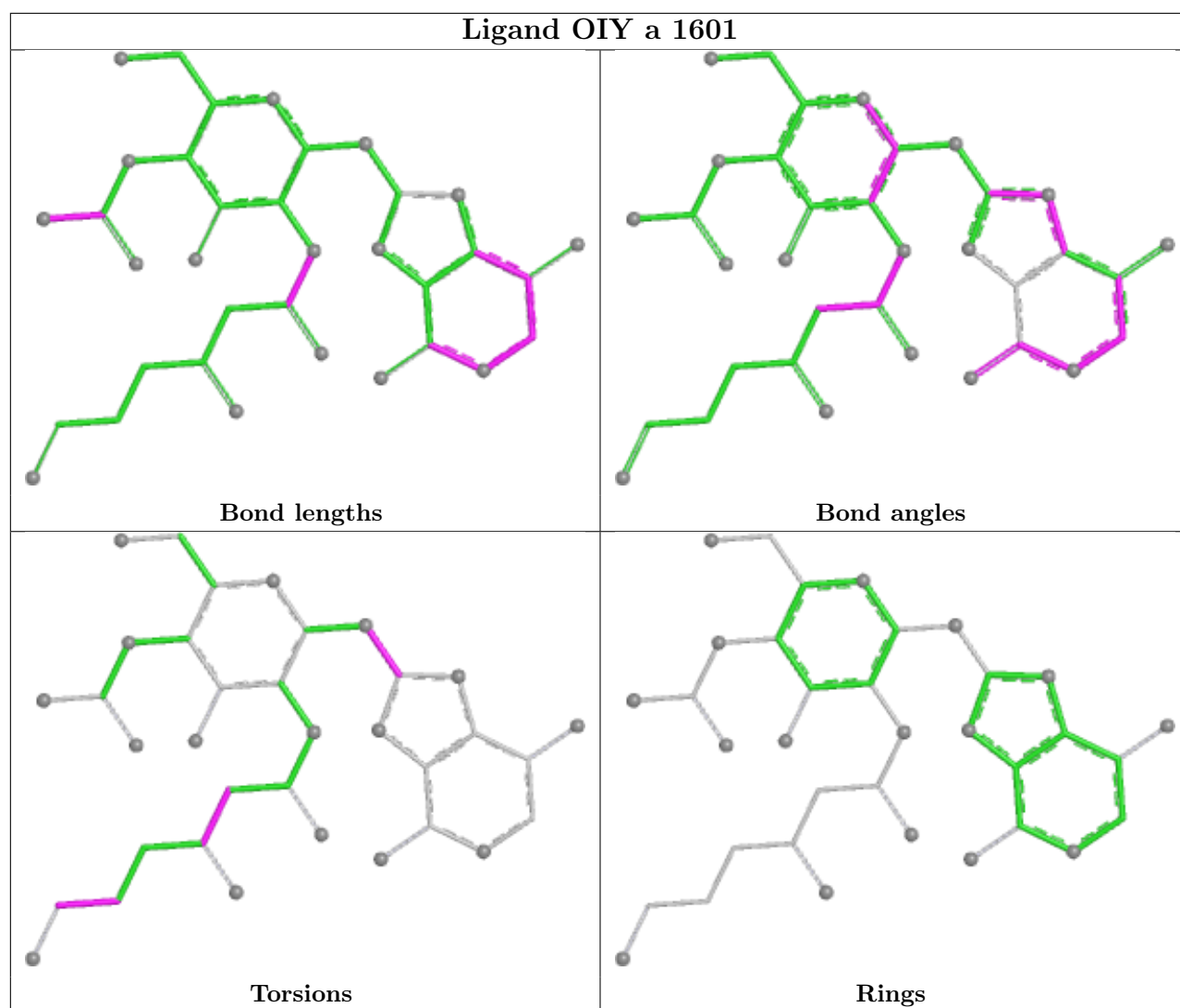
There are no ring outliers.

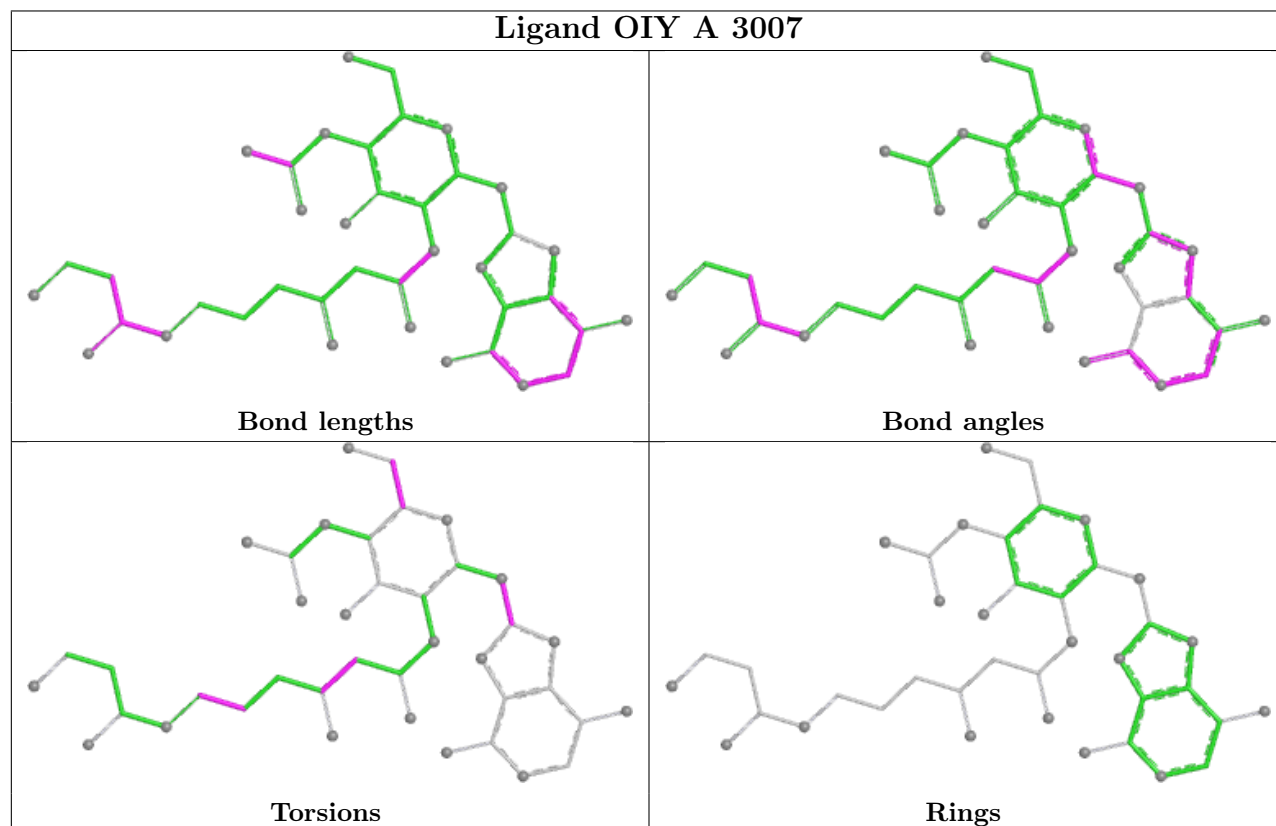
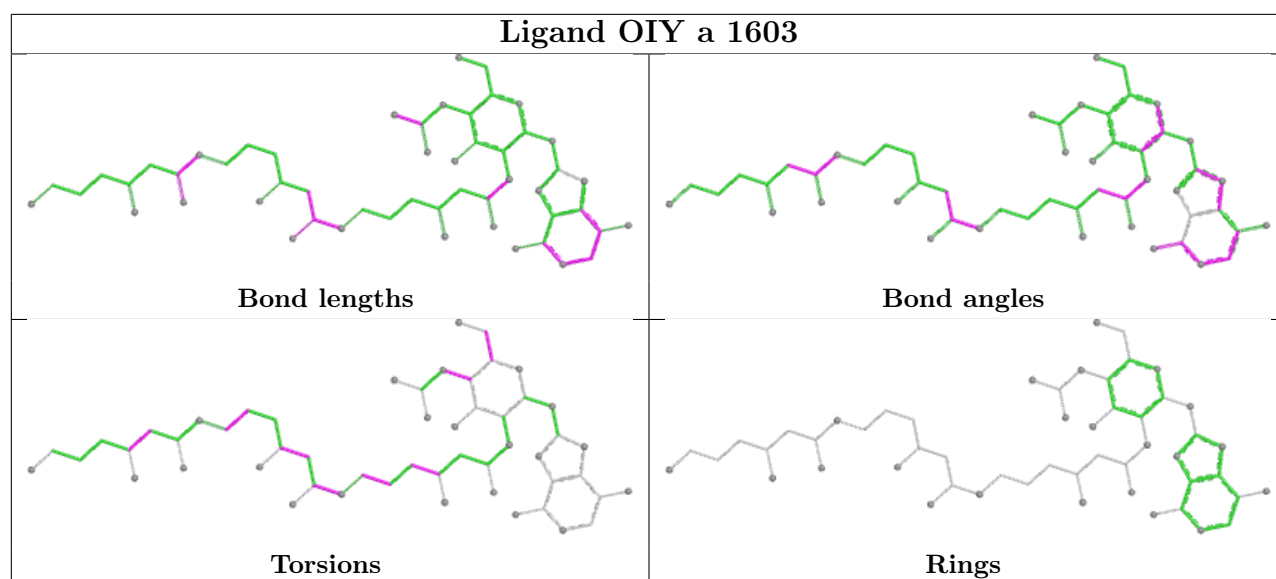
7 monomers are involved in 8 short contacts:

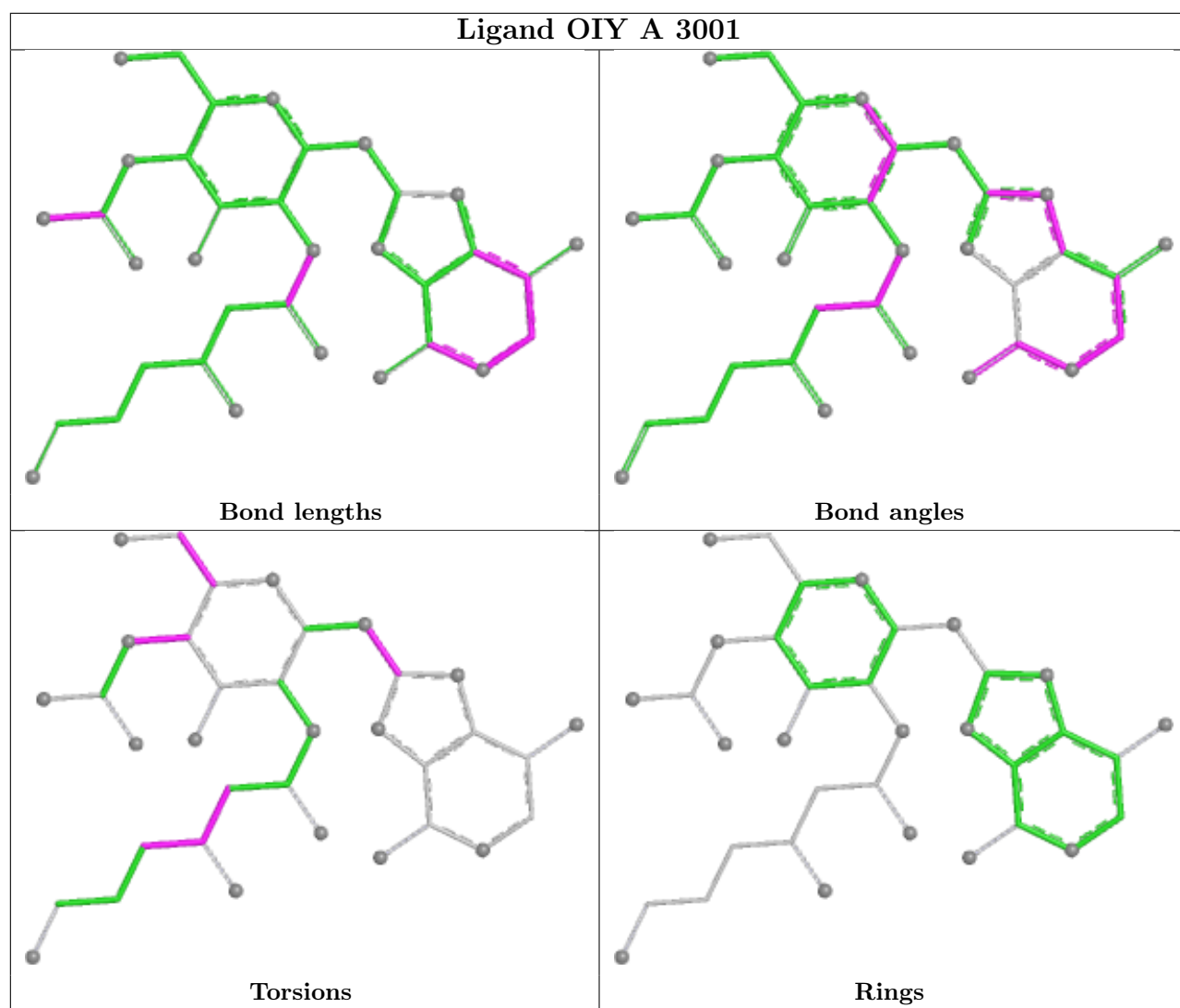
Mol	Chain	Res	Type	Clashes	Symm-Clashes
53	a	1601	OIY	2	0
53	A	3005	OIY	1	0
53	A	3003	OIY	1	0
53	a	1602	OIY	1	0
53	W	101	OIY	1	0
53	A	3006	OIY	1	0
53	A	3002	OIY	1	0

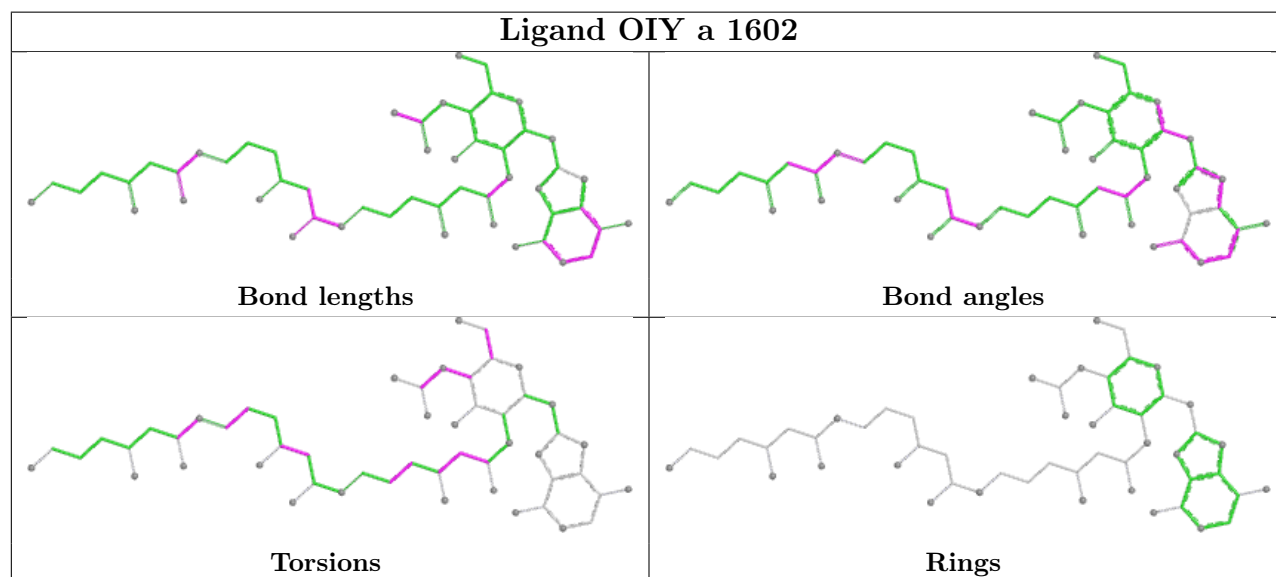
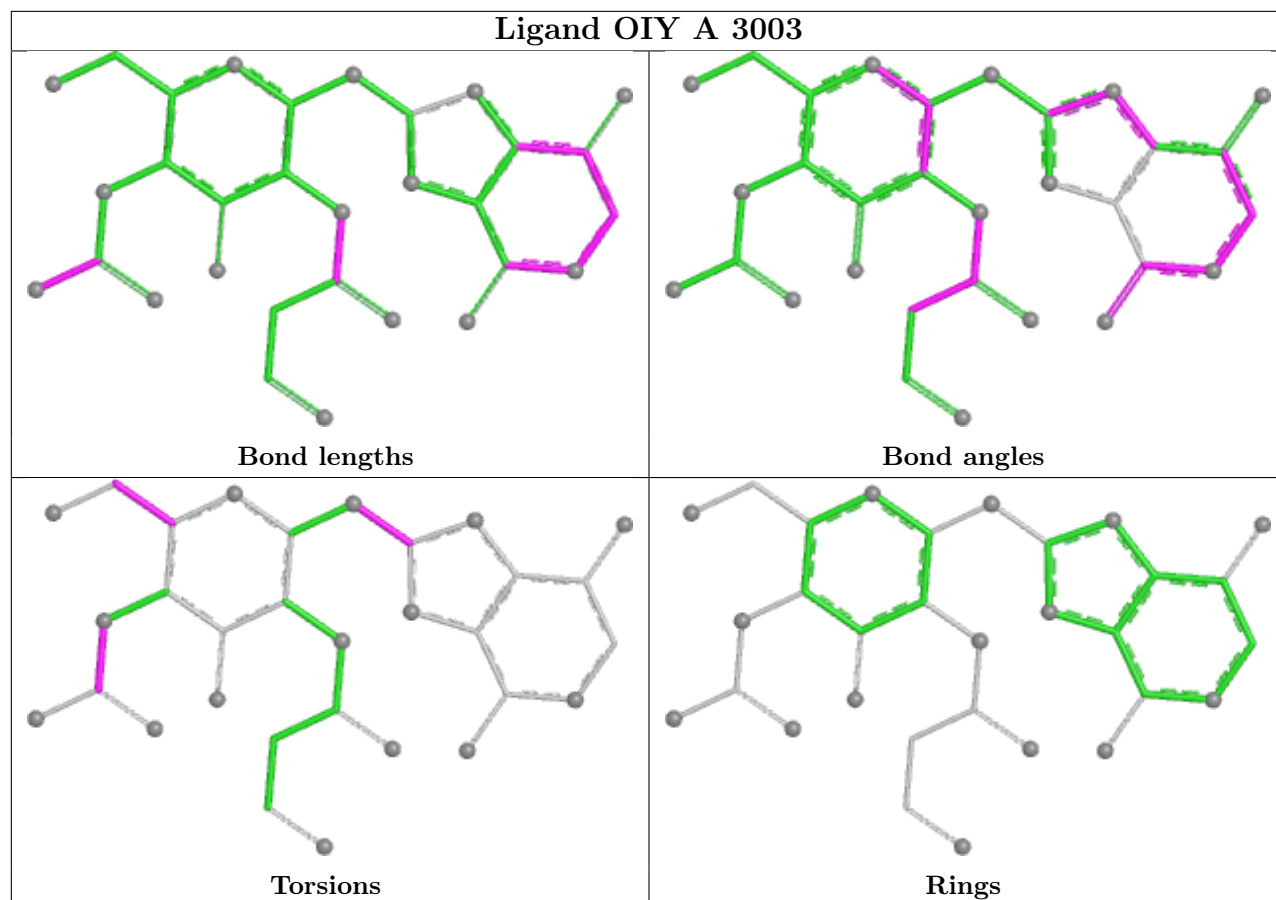
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

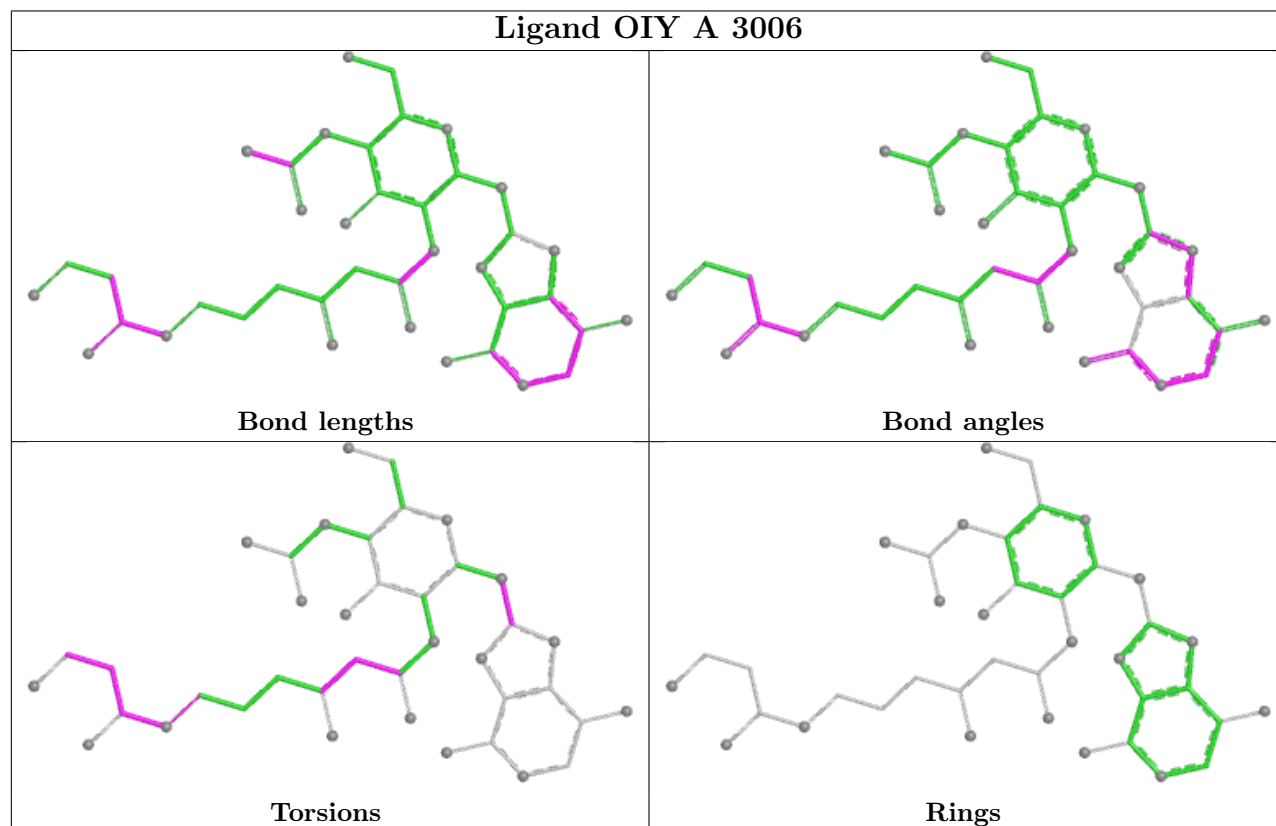
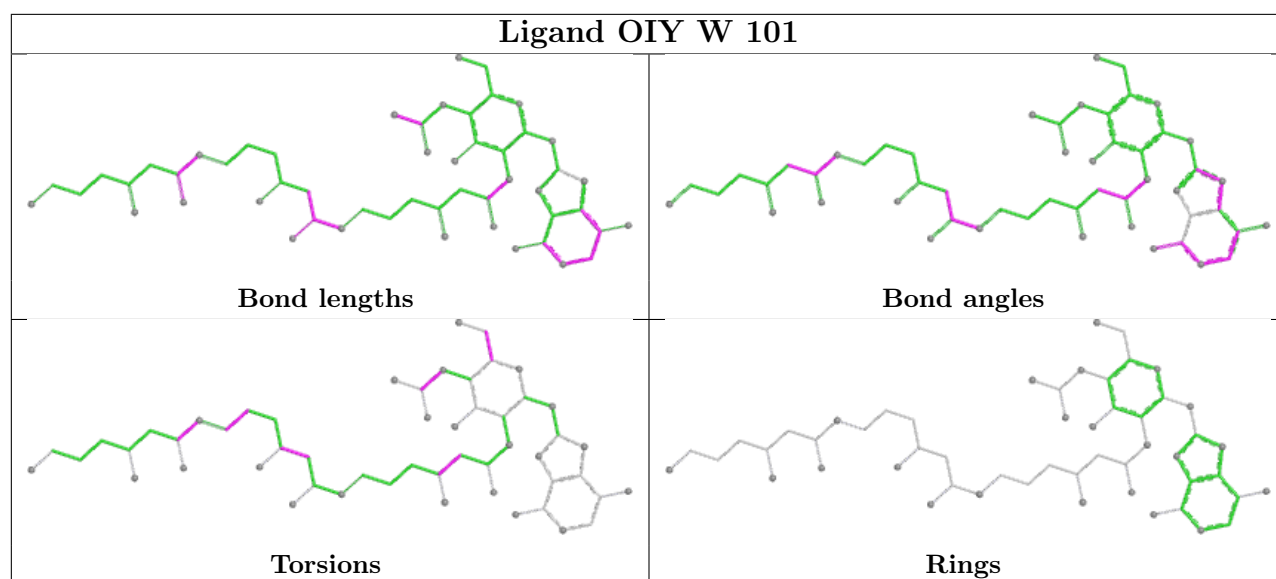


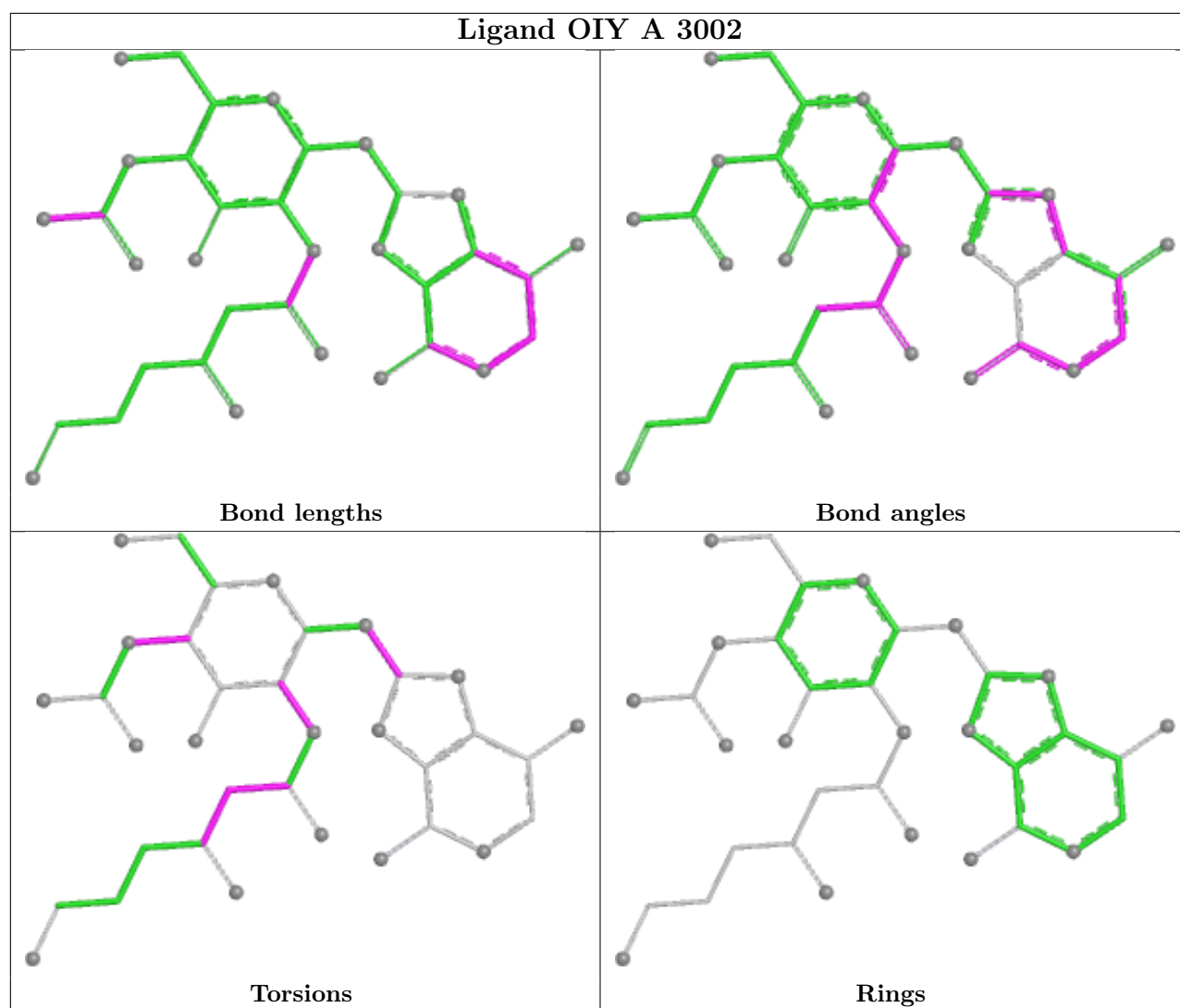












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

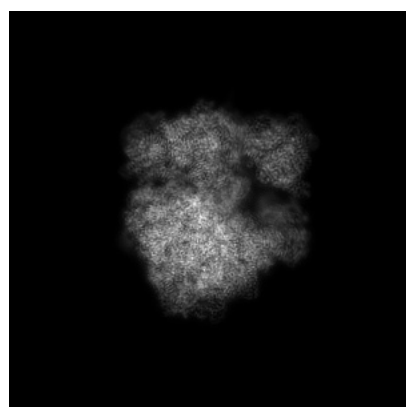
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26822. These allow visual inspection of the internal detail of the map and identification of artifacts.

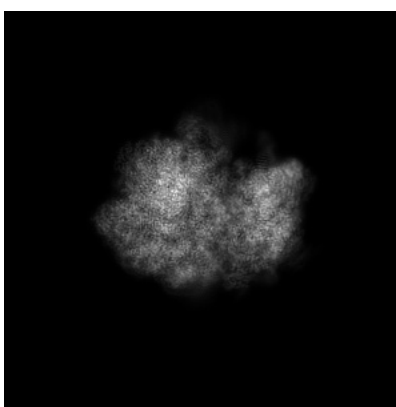
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

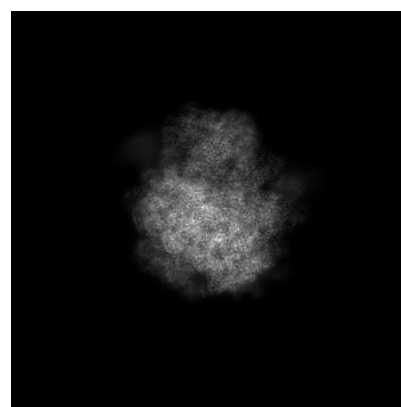
6.1.1 Primary map



X



Y



Z

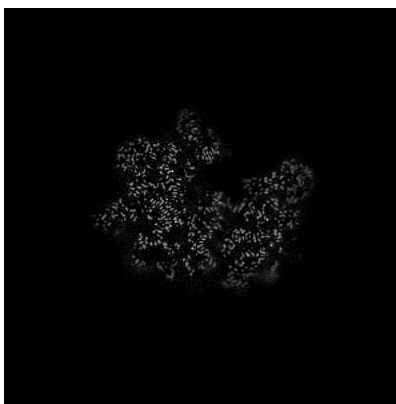
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

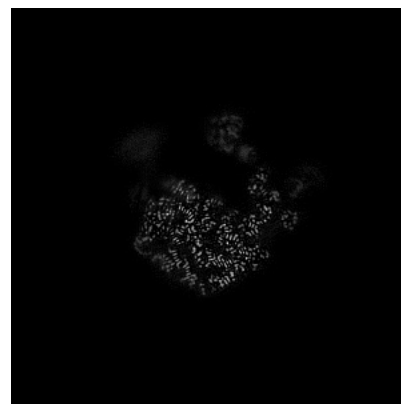
6.2.1 Primary map



X Index: 320



Y Index: 320

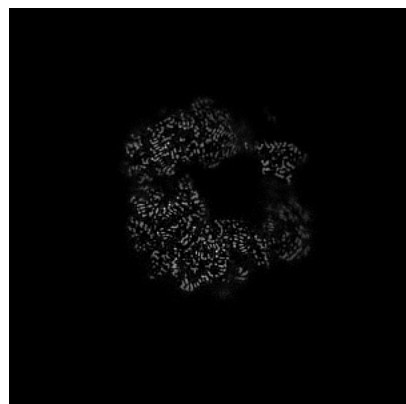


Z Index: 320

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

6.3 Largest variance slices [i](#)

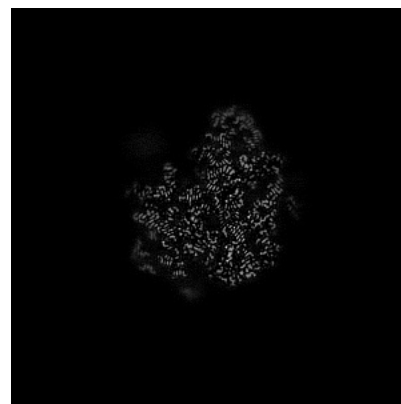
6.3.1 Primary map



X Index: 353



Y Index: 303

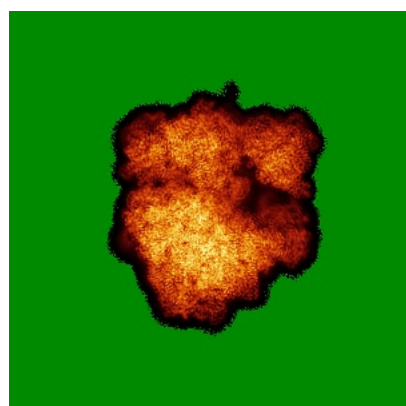


Z Index: 276

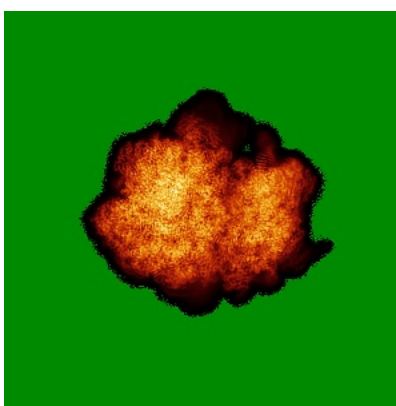
The images above show the largest variance slices of the map in three orthogonal directions.

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

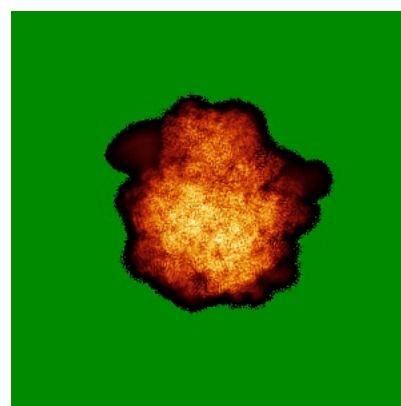
6.4.1 Primary map



X



Y



Z

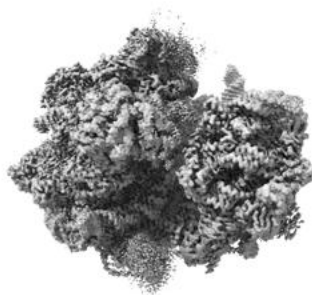
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

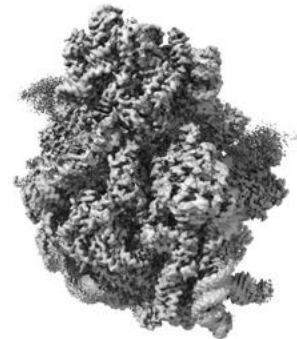
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

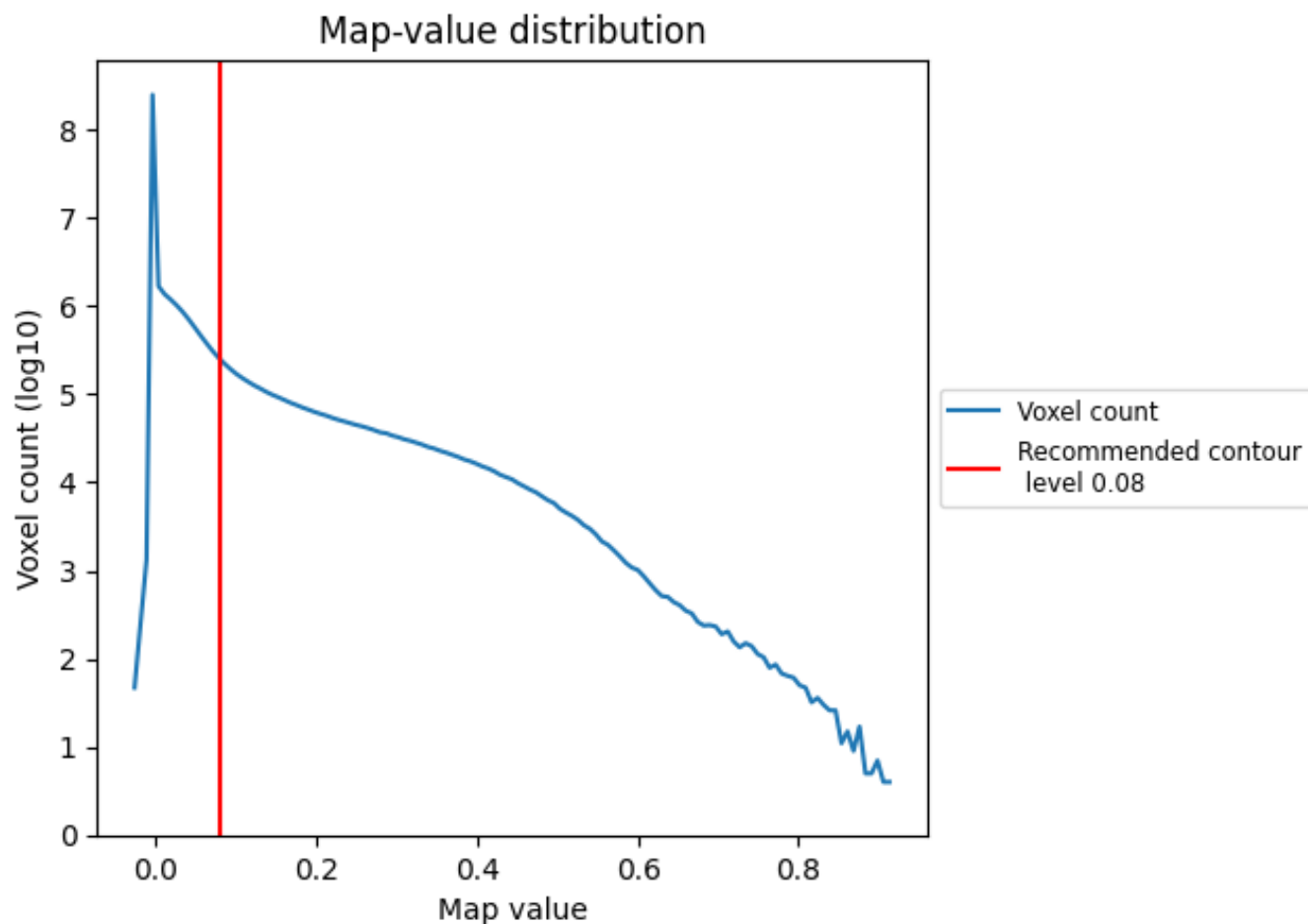
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

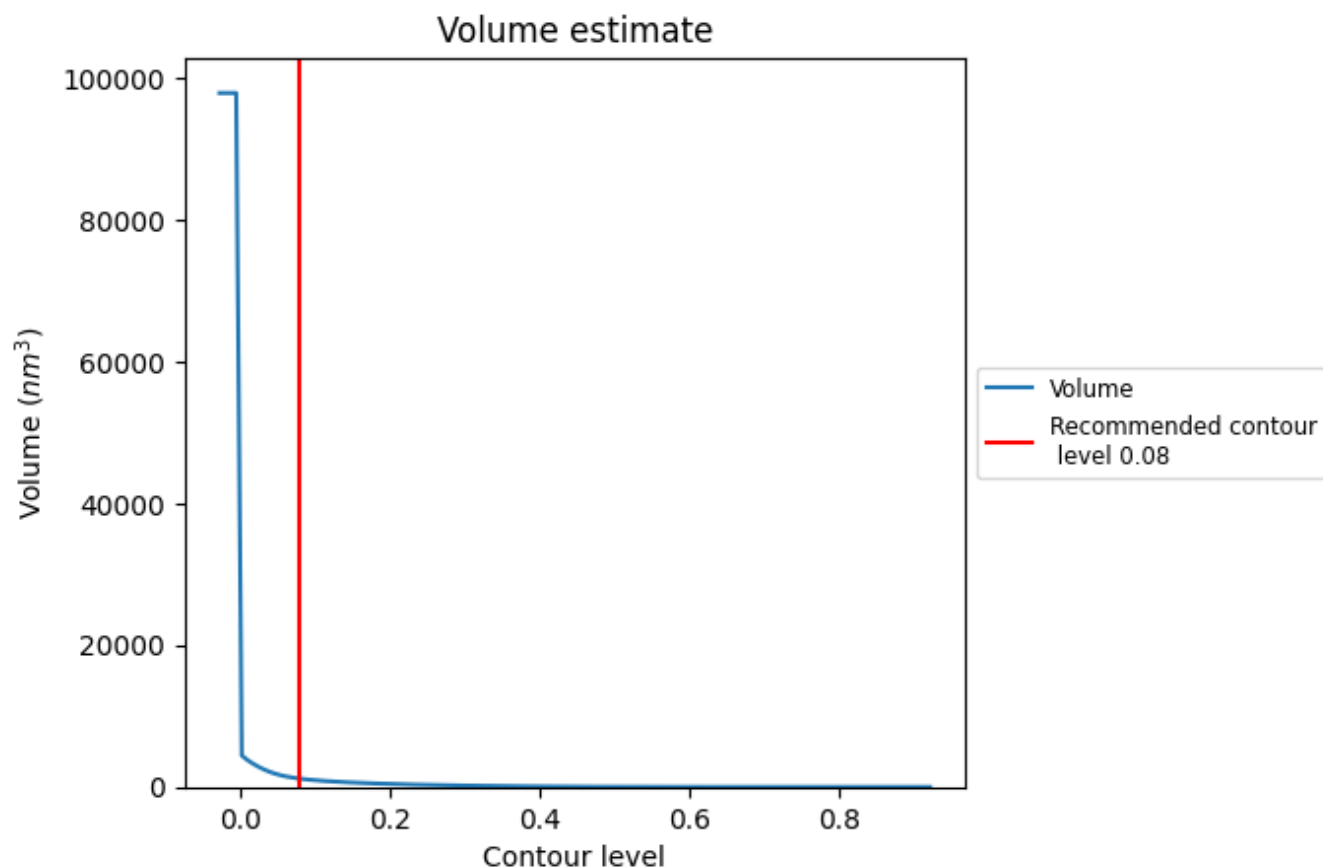
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

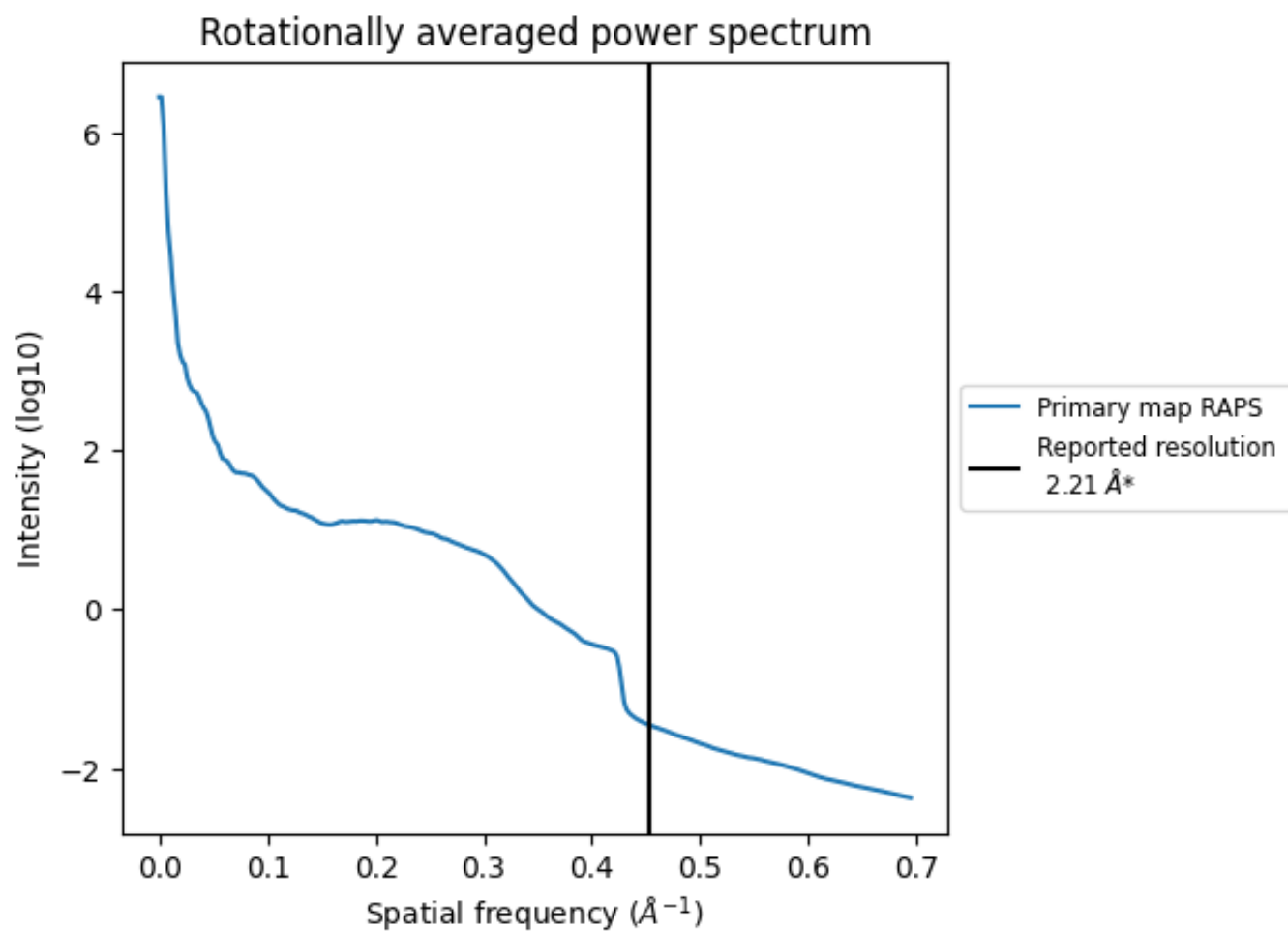
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1178 nm^3 ; this corresponds to an approximate mass of 1064 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 0.452 Å⁻¹

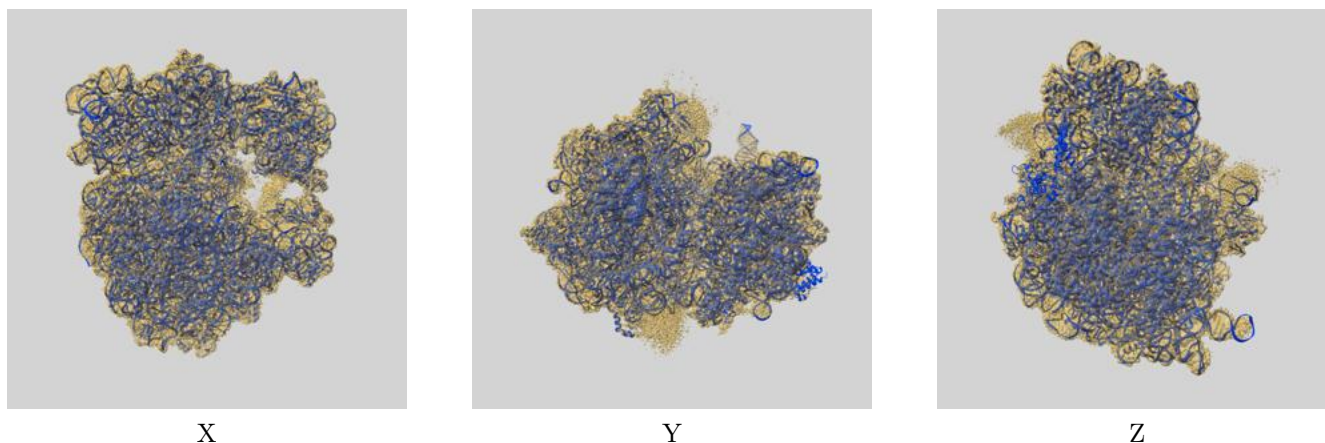
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

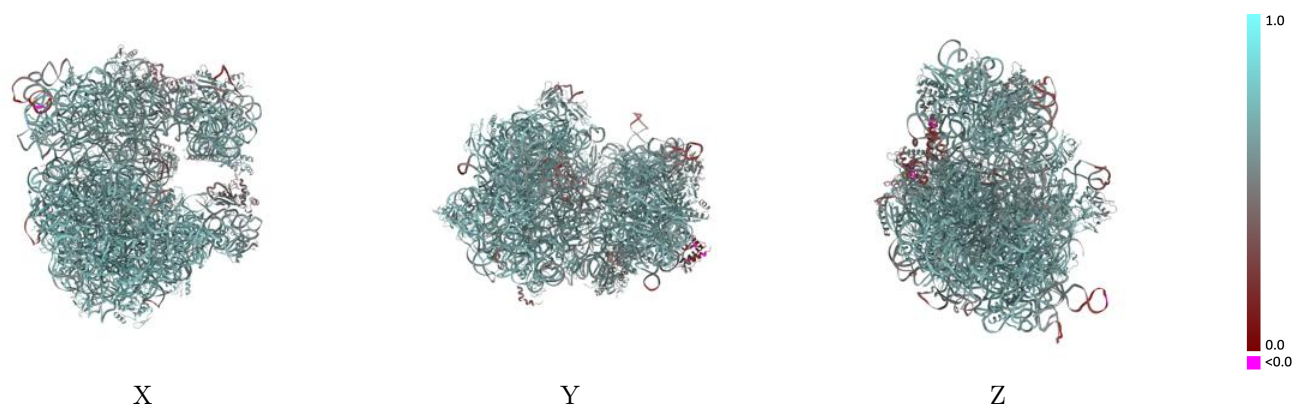
This section contains information regarding the fit between EMDB map EMD-26822 and PDB model 7UW1. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



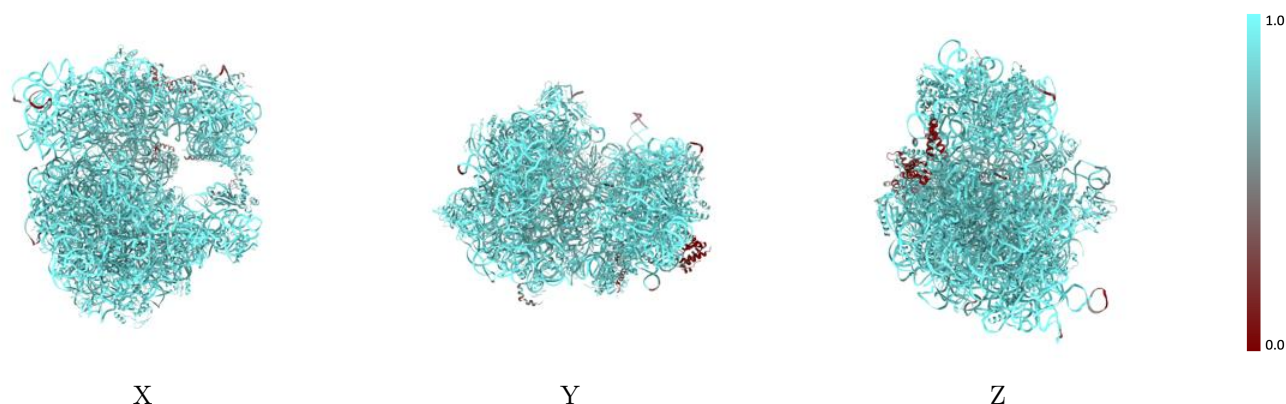
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



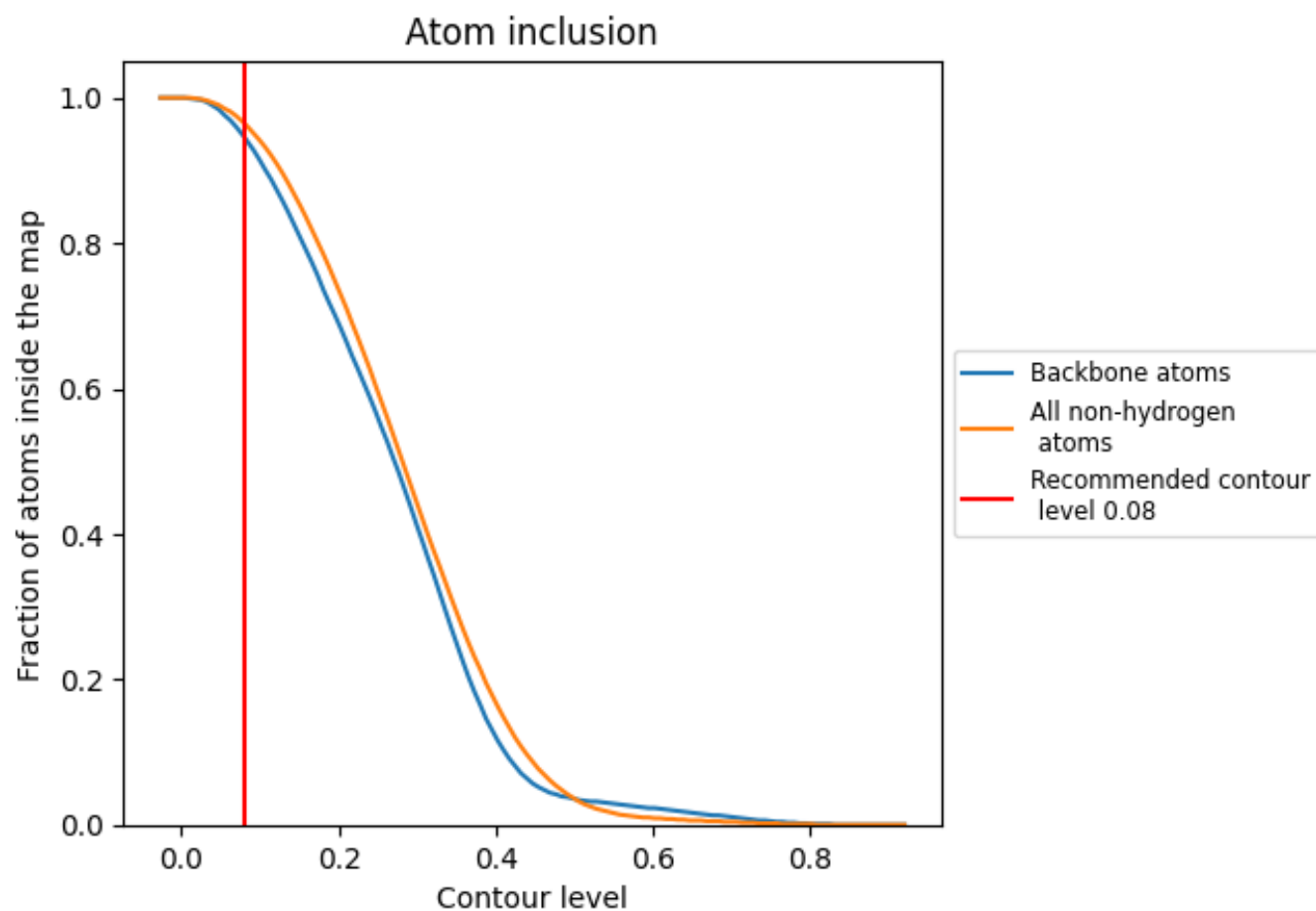
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 96% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9650	 0.6390
0	 0.9330	 0.6650
1	 0.9940	 0.7270
2	 0.9980	 0.7120
3	 0.9790	 0.6830
A	 0.9870	 0.6600
B	 0.9930	 0.5980
C	 0.9890	 0.6990
D	 0.9840	 0.7050
E	 0.9750	 0.6880
F	 0.7690	 0.4320
G	 0.9110	 0.5870
H	 0.7370	 0.5050
I	 0.9890	 0.7010
J	 0.9800	 0.6860
K	 0.9840	 0.6960
L	 0.9740	 0.6850
M	 0.9970	 0.7150
N	 0.9640	 0.6130
O	 0.9720	 0.6830
P	 1.0000	 0.7180
Q	 0.9760	 0.6930
R	 0.9910	 0.7100
S	 0.9640	 0.6600
T	 0.9350	 0.6370
U	 0.9570	 0.6590
V	 0.9890	 0.7040
W	 0.9630	 0.6760
X	 0.9370	 0.6210
Y	 0.9750	 0.6940
Z	 0.9740	 0.6990
a	 0.9820	 0.6150
b	 0.3840	 0.3910
c	 0.9320	 0.6180
d	 0.9180	 0.5530



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Chain	Atom inclusion	Q-score
e	 0.9770	 0.6400
f	 0.9130	 0.5770
g	 0.7790	 0.5140
h	 0.9790	 0.6590
i	 0.9490	 0.6290
j	 0.8990	 0.6090
k	 0.9060	 0.5590
l	 0.9330	 0.6240
m	 0.9590	 0.6270
n	 0.9500	 0.6400
o	 0.9780	 0.6410
p	 0.9820	 0.6620
q	 0.9690	 0.6350
r	 0.9760	 0.6220
s	 0.9680	 0.6350
t	 0.9780	 0.6470
u	 0.5490	 0.5000