



Full wwPDB EM Validation Report ⓘ

Jun 18, 2026 – 02:23 pm BST

PDB ID : 7NWT / pdb_00007nwt
EMDB ID : EMD-12635
Title : Initiated 70S ribosome in complex with 2A protein from encephalomyocarditis virus (EMCV)
Authors : Hill, C.H.; Naphine, S.; Pekarek, L.; Kibe, A.; Firth, A.E.; Graham, S.C.; Caliskan, N.; Brierley, I.
Deposited on : 2021-03-17
Resolution : 2.66 Å (reported)
Based on initial model : 5MDZ

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:

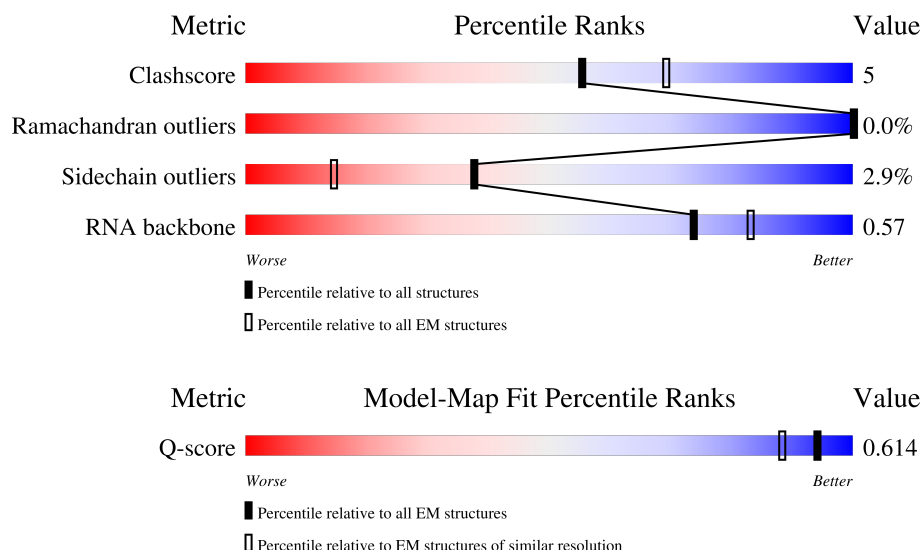
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.66 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.



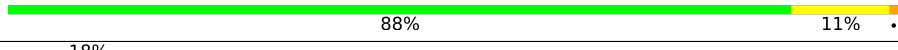
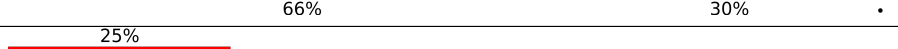
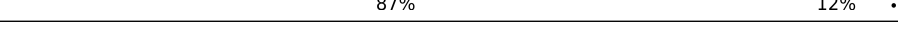
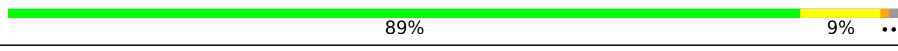
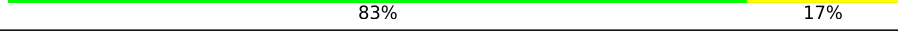
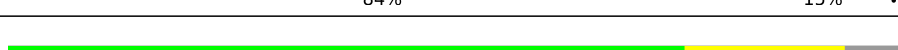
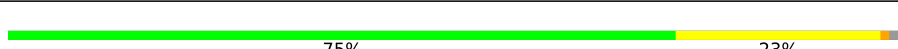
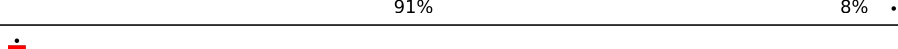
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	9119 (2.16 - 3.16)

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

Mol	Chain	Length	Quality of chain
1	B	273	 85% 14% ..
2	C	209	 91% 8% .
3	D	201	 86% 13%

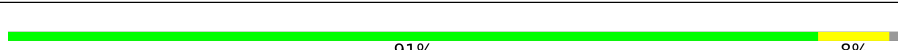
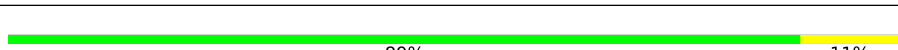
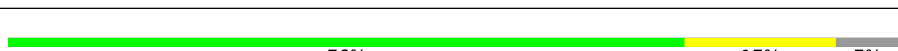
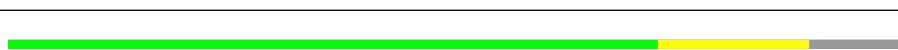
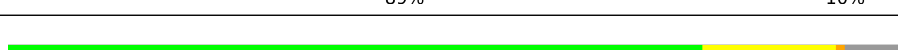
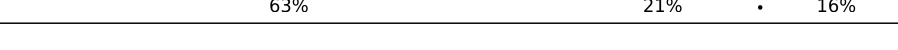
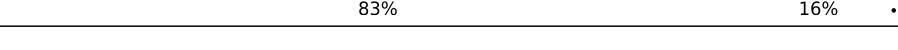
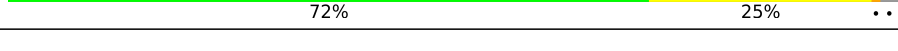
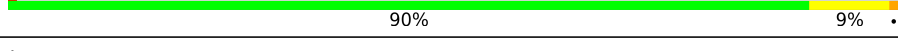
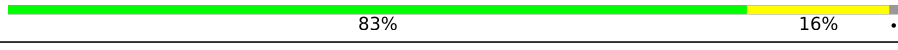
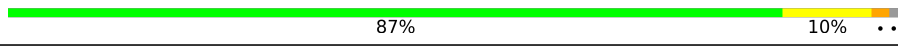
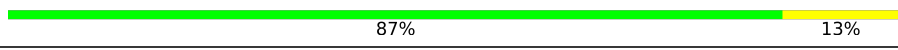
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Mol	Chain	Length	Quality of chain
4	E	179	
5	F	177	
6	G	149	
7	H	165	
8	I	142	
9	J	142	
10	K	123	
11	L	144	
12	M	136	
13	N	127	
14	O	117	
15	P	115	
16	Q	118	
17	R	103	
18	S	110	
19	T	100	
20	U	104	
21	V	94	
22	W	85	
23	X	78	
24	Y	63	
25	Z	59	
26	1	2904	
27	2	1534	
28	3	120	

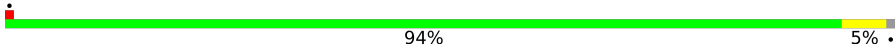
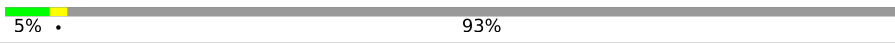
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Mol	Chain	Length	Quality of chain
29	5	77	
30	a	70	
31	b	57	
32	c	55	
33	d	46	
34	e	65	
35	f	38	
36	g	241	
37	h	233	
38	i	206	
39	j	167	
40	k	135	
41	l	179	
42	m	130	
43	n	130	
44	o	103	
45	p	129	
46	q	124	
47	r	118	
48	s	101	
49	t	89	
50	u	82	
51	v	84	
52	w	75	
53	x	92	

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Mol	Chain	Length	Quality of chain
54	y	87	
55	z	71	
56	XX	117	
57	AA	152	
57	BB	152	
57	CC	152	

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 149932 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 L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 2 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 3 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 4 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 5 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	175	Total	C	N	O	S	0	0
			1313	826	241	244	2		

- Molecule 6 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 7 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	130	Total	C	N	O	S	0	0
			980	620	174	182	4		

- Molecule 8 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	135	Total	C	N	O	S	0	0
			984	622	171	185	6		

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	119	Total	C	N	O	S	0	0
			951	588	195	163	5		

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	O	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	Q	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	94	Total	C	N	O	S	0	0
			746	470	140	134	2		

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	U	103	Total	C	N	O	0	0
			788	498	148	142		

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	76	Total	C	N	O	S	0	0
			582	360	117	104	1		

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	58	Total	C	N	O	S	0	0
			448	281	87	78	2		

- Molecule 26 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	1	2903	Total	C	N	O	P	0	0
			62336	27816	11470	20147	2903		

- Molecule 27 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	2	1534	Total	C	N	O	P	0	0
			32929	14693	6041	10661	1534		

- Molecule 28 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	3	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 29 is a RNA chain called fMet-NH-tRNA(fMet).

Mol	Chain	Residues	Atoms					AltConf	Trace	
29	5	76	Total	C	N	O	P	S	0	0
			1622	725	292	528	76	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	8	4SU	G	conflict	GB 1317722521

- Molecule 30 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	a	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 31 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	b	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 32 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	c	52	Total	C	N	O	0	0
			426	275	78	73		

- Molecule 33 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	d	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 34 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	e	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 35 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	f	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 36 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	g	225	Total	C	N	O	S	0	0
			1760	1113	316	323	8		

- Molecule 37 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	h	208	Total	C	N	O	S	0	0
			1636	1036	307	290	3		

- Molecule 38 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	i	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 39 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	j	156	Total	C	N	O	S	0	0
			1152	717	217	212	6		

- Molecule 40 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	k	104	Total	C	N	O	S	0	0
			848	536	153	152	7		

- Molecule 41 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 42 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	m	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 43 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	n	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 44 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	o	99	Total	C	N	O	S	0	0
			790	495	151	143	1		

- Molecule 45 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	p	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 46 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	q	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

- Molecule 47 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	r	116	Total	C	N	O	S	0	0
			900	558	181	158	3		

- Molecule 48 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	s	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 49 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	t	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 50 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	u	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 51 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	v	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 52 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	w	66	Total	C	N	O	S	0	0
			544	344	102	97	1		

- Molecule 53 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	x	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

- Molecule 54 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	y	86	Total	C	N	O	S	0	0
			669	414	138	114	3		

- Molecule 55 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	z	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 56 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	XX	8	Total	C	N	O	P	0	0
			176	78	34	56	8		

- Molecule 57 is a protein called Protein 2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	AA	127	Total	C	N	O	S	0	0
			1067	690	192	182	3		
57	BB	130	Total	C	N	O	S	2	0
			1111	716	204	188	3		
57	CC	125	Total	C	N	O	S	0	0
			1048	677	190	178	3		

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	144	GLY	-	expression tag	UNP P12296
AA	145	SER	-	expression tag	UNP P12296
AA	146	LYS	-	expression tag	UNP P12296
AA	147	HIS	-	expression tag	UNP P12296
AA	148	HIS	-	expression tag	UNP P12296
AA	149	HIS	-	expression tag	UNP P12296
AA	150	HIS	-	expression tag	UNP P12296
AA	151	HIS	-	expression tag	UNP P12296
AA	152	HIS	-	expression tag	UNP P12296
BB	144	GLY	-	expression tag	UNP P12296
BB	145	SER	-	expression tag	UNP P12296
BB	146	LYS	-	expression tag	UNP P12296
BB	147	HIS	-	expression tag	UNP P12296
BB	148	HIS	-	expression tag	UNP P12296
BB	149	HIS	-	expression tag	UNP P12296
BB	150	HIS	-	expression tag	UNP P12296
BB	151	HIS	-	expression tag	UNP P12296
BB	152	HIS	-	expression tag	UNP P12296
CC	144	GLY	-	expression tag	UNP P12296
CC	145	SER	-	expression tag	UNP P12296
CC	146	LYS	-	expression tag	UNP P12296

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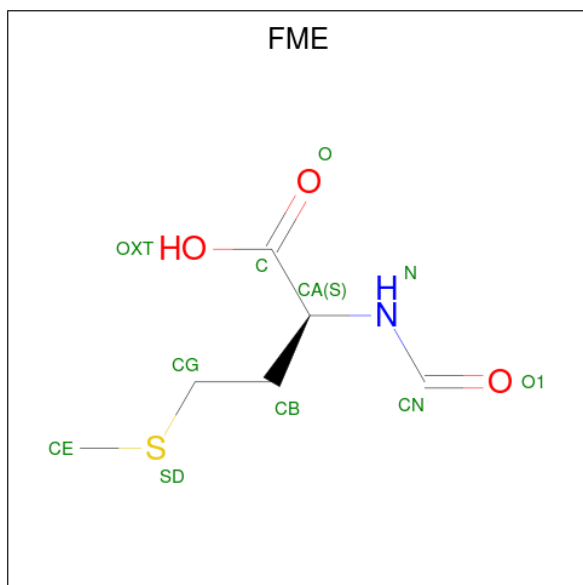
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Chain	Residue	Modelled	Actual	Comment	Reference
CC	147	HIS	-	expression tag	UNP P12296
CC	148	HIS	-	expression tag	UNP P12296
CC	149	HIS	-	expression tag	UNP P12296
CC	150	HIS	-	expression tag	UNP P12296
CC	151	HIS	-	expression tag	UNP P12296
CC	152	HIS	-	expression tag	UNP P12296

- Molecule 58 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
58	B	1	Total Mg 1 1	0
58	C	1	Total Mg 1 1	0
58	M	1	Total Mg 1 1	0
58	N	1	Total Mg 1 1	0
58	Q	1	Total Mg 1 1	0
58	1	290	Total Mg 290 290	0
58	2	128	Total Mg 128 128	0
58	3	8	Total Mg 8 8	0
58	5	3	Total Mg 3 3	0
58	b	1	Total Mg 1 1	0
58	i	1	Total Mg 1 1	0
58	BB	1	Total Mg 1 1	0

- Molecule 59 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: C₆H₁₁NO₃S).



Mol	Chain	Residues	Atoms					AltConf
59	5	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
60	a	1	Total	Zn	0
			1	1	
60	f	1	Total	Zn	0
			1	1	

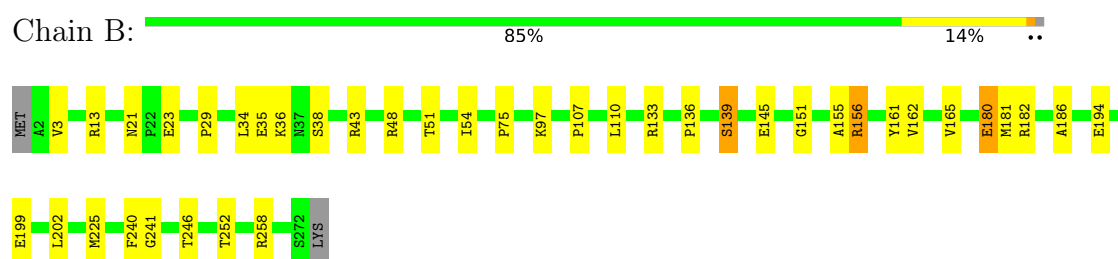
- Molecule 61 is water.

Mol	Chain	Residues	Atoms		AltConf
61	B	2	Total	O	0
			2	2	

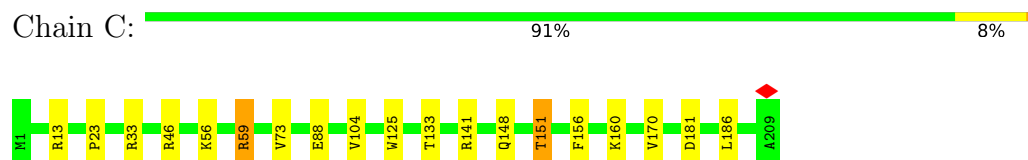
3 Residue-property plots

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

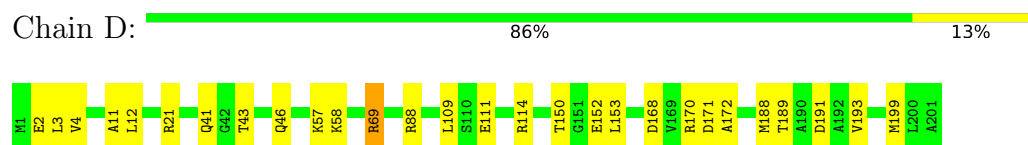
• Molecule 1: 50S ribosomal protein L2



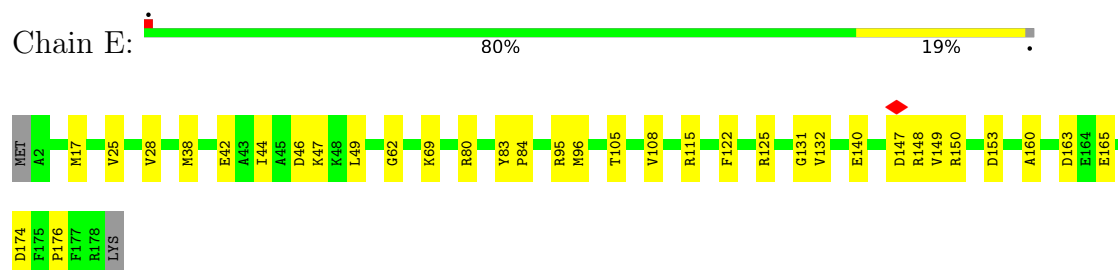
• Molecule 2: 50S ribosomal protein L3



• Molecule 3: 50S ribosomal protein L4



• Molecule 4: 50S ribosomal protein L5



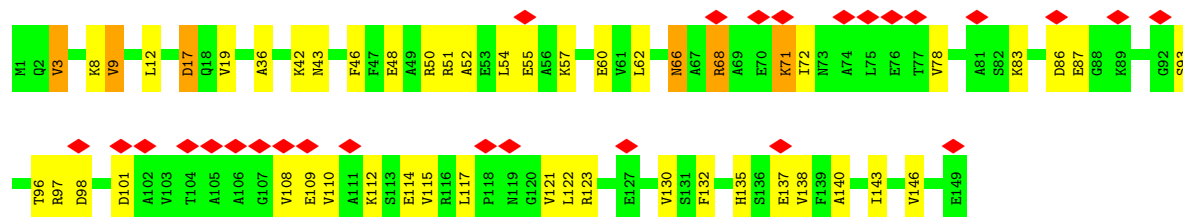
• Molecule 5: 50S ribosomal protein L6

Chain F: 



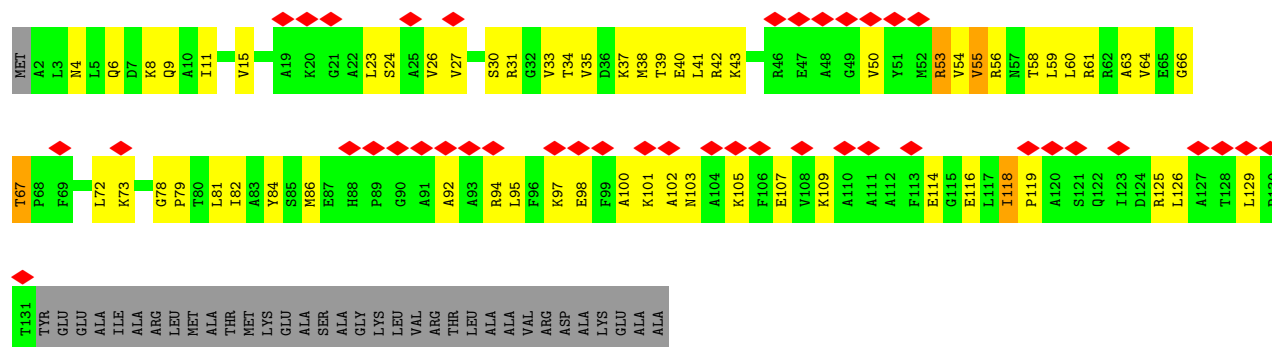
- Molecule 6: 50S ribosomal protein L9

Chain G: 



- Molecule 7: 50S ribosomal protein L10

Chain H: 



- Molecule 8: 50S ribosomal protein L11

Chain I: 



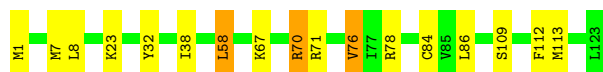
- Molecule 9: 50S ribosomal protein L13

Chain J: 



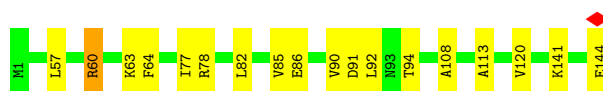
- Molecule 10: 50S ribosomal protein L14

Chain K: 86% 11% .



- Molecule 11: 50S ribosomal protein L15

Chain L: 88% 12% .



- Molecule 12: 50S ribosomal protein L16

Chain M: 87% 12% .



- Molecule 13: 50S ribosomal protein L17

Chain N: 85% 8% 6%



- Molecule 14: 50S ribosomal protein L18

Chain O: 93% 6% .



- Molecule 15: 50S ribosomal protein L19

Chain P: 83% 15% ..



- Molecule 16: 50S ribosomal protein L20

Chain Q: 89% 9% ..



- Molecule 17: 50S ribosomal protein L21

Chain R: 83% 17%



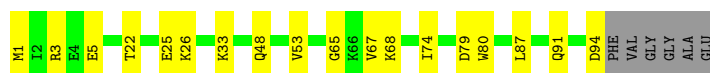
- Molecule 18: 50S ribosomal protein L22

Chain S: 84% 15%



- Molecule 19: 50S ribosomal protein L23

Chain T: 76% 18% 6%



- Molecule 20: 50S ribosomal protein L24

Chain U: 75% 23%



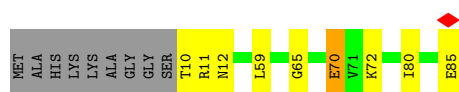
- Molecule 21: 50S ribosomal protein L25

Chain V: 89% 11%



- Molecule 22: 50S ribosomal protein L27

Chain W: 79% 9% 11%

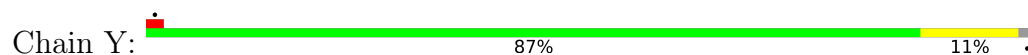


- Molecule 23: 50S ribosomal protein L28

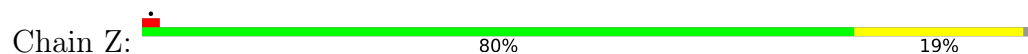
Chain X: 91% 8%



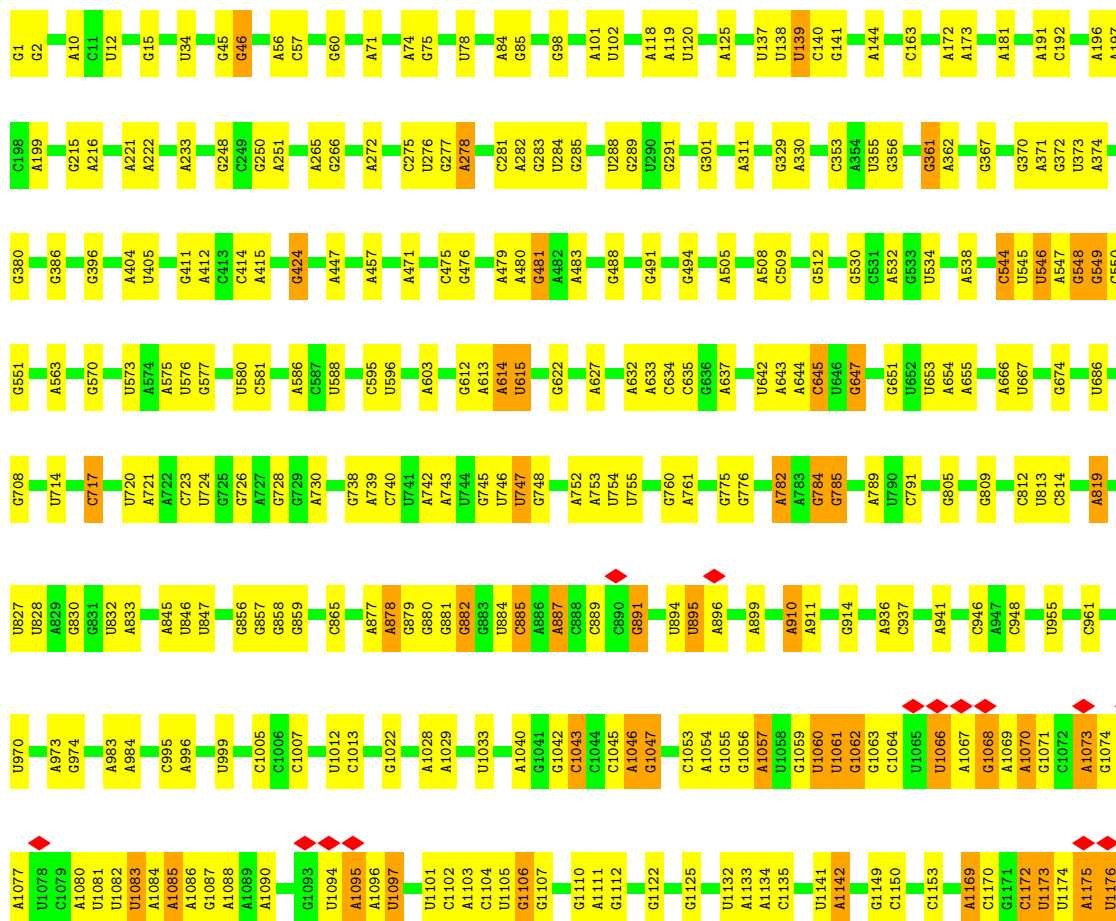
- Molecule 24: 50S ribosomal protein L29

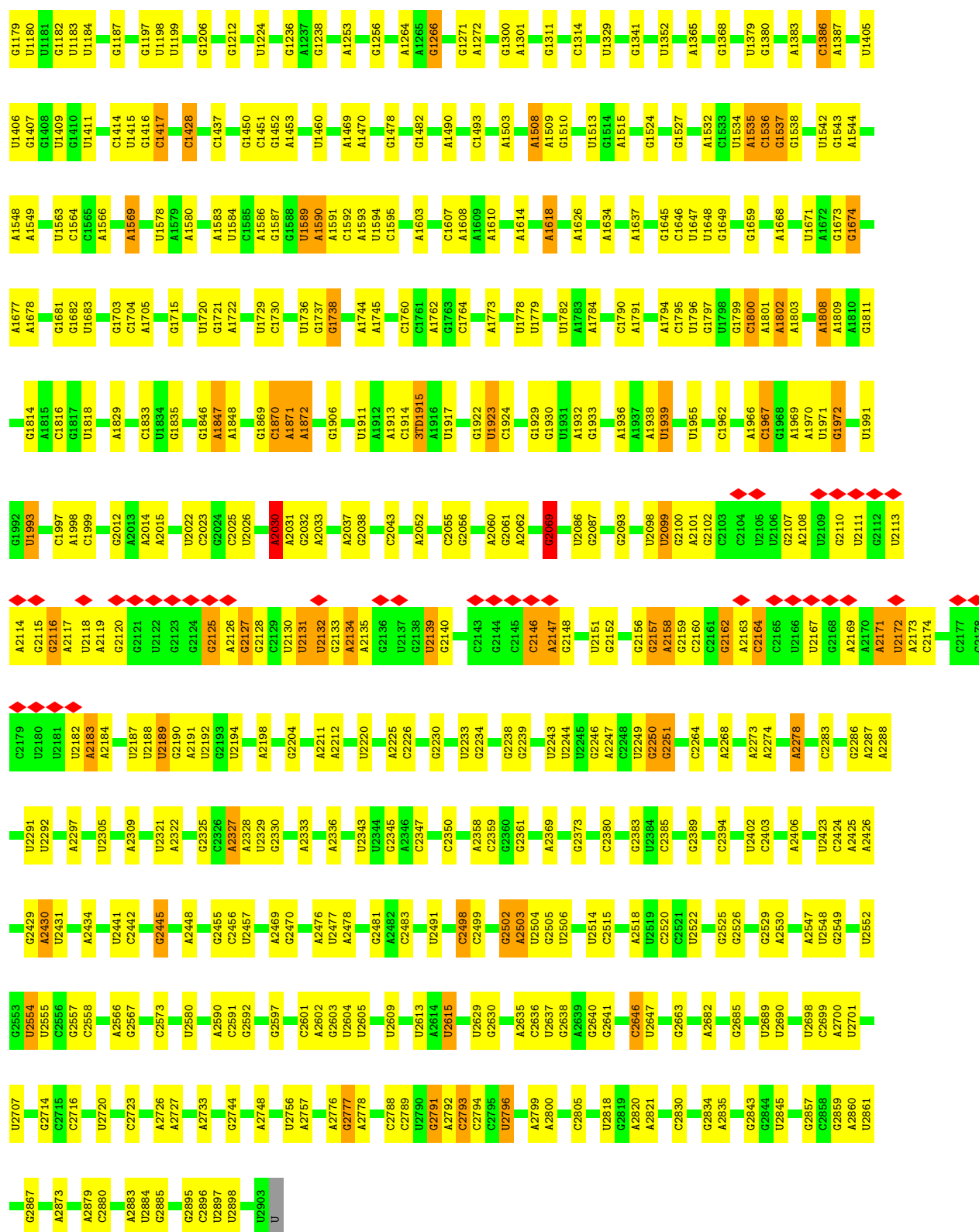


- Molecule 25: 50S ribosomal protein L30



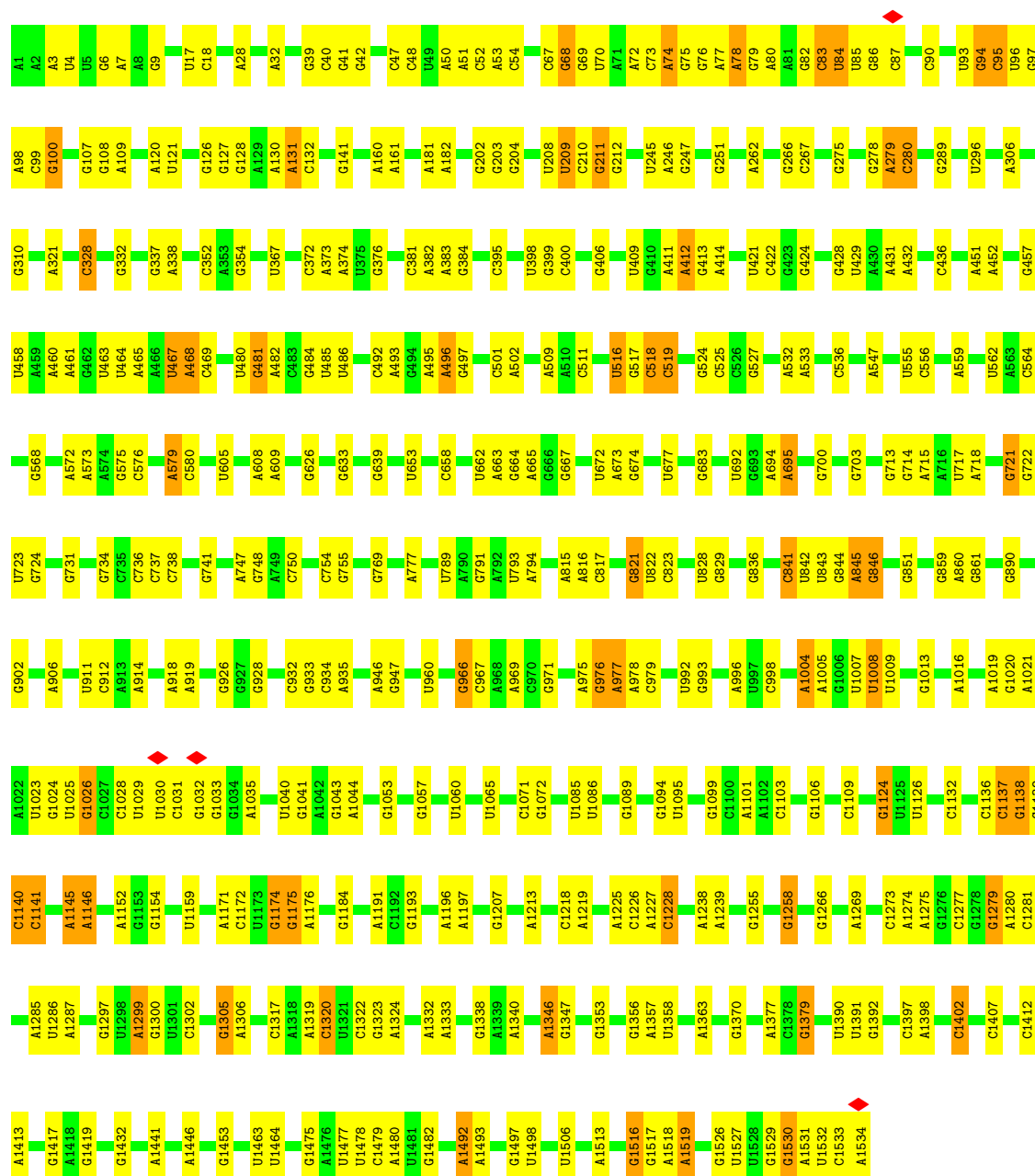
- Molecule 26: 23S ribosomal RNA





• Molecule 27: 16S ribosomal RNA

Chain 2:



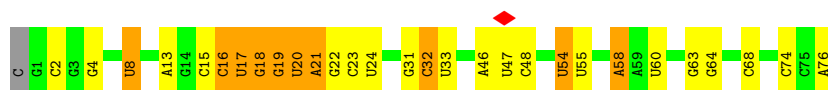
• Molecule 28: 5S ribosomal RNA

Chain 3: 81% 18%



• Molecule 29: fMet-NH-tRNA(fMet)

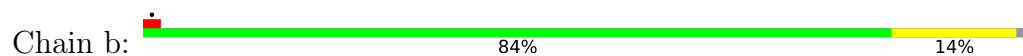
Chain 5: 61% 25% 13%



- Molecule 30: 50S ribosomal protein L31



- Molecule 31: 50S ribosomal protein L32



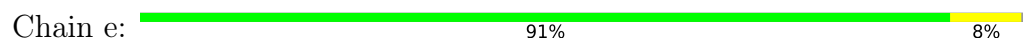
- Molecule 32: 50S ribosomal protein L33



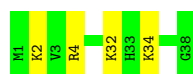
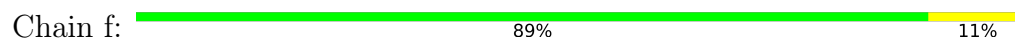
- Molecule 33: 50S ribosomal protein L34



- Molecule 34: 50S ribosomal protein L35

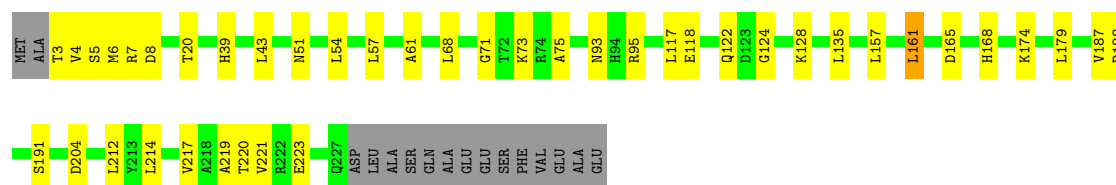


- Molecule 35: 50S ribosomal protein L36



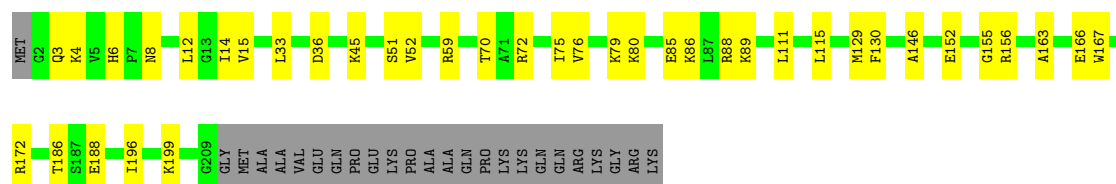
- Molecule 36: 30S ribosomal protein S2

Chain g: 



- Molecule 37: 30S ribosomal protein S3

Chain h: 



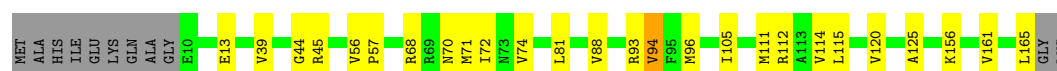
- Molecule 38: 30S ribosomal protein S4

Chain i: 



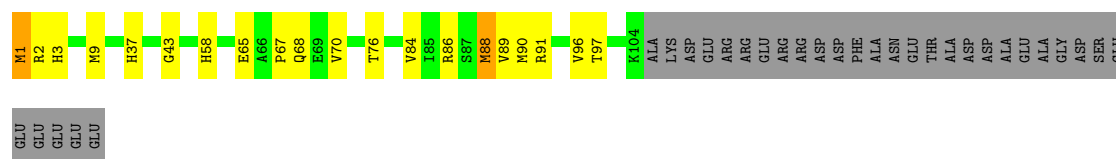
- Molecule 39: 30S ribosomal protein S5

Chain j: 



- Molecule 40: 30S ribosomal protein S6

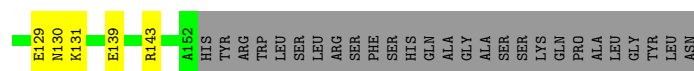
Chain k: 



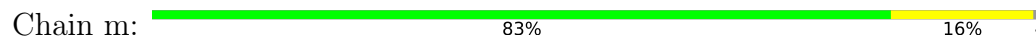
- Molecule 41: 30S ribosomal protein S7

Chain l: 

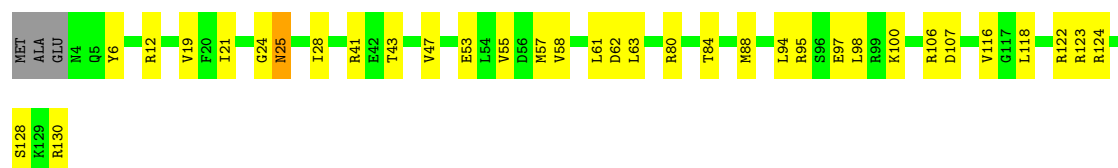




- Molecule 42: 30S ribosomal protein S8



- Molecule 43: 30S ribosomal protein S9



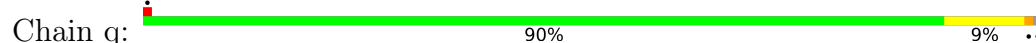
- Molecule 44: 30S ribosomal protein S10



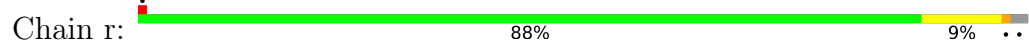
- Molecule 45: 30S ribosomal protein S11



- Molecule 46: 30S ribosomal protein S12



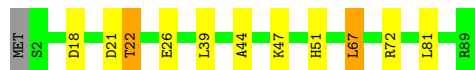
- Molecule 47: 30S ribosomal protein S13



• Molecule 48: 30S ribosomal protein S14

Chain s:  83% 16%

• Molecule 49: 30S ribosomal protein S15

Chain t:  87% 10%

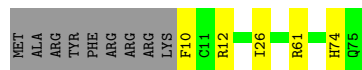
• Molecule 50: 30S ribosomal protein S16

Chain u:  87% 13%

• Molecule 51: 30S ribosomal protein S17

Chain v:  85% 11% 5%

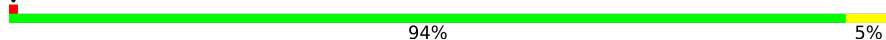
• Molecule 52: 30S ribosomal protein S18

Chain w:  81% 7% 12%

• Molecule 53: 30S ribosomal protein S19

Chain x:  68% 21% 10%

• Molecule 54: 30S ribosomal protein S20

Chain y:  94% 5%

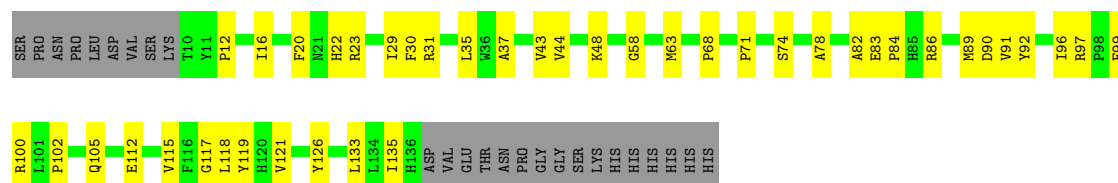
Chain z:



Chain XX: 5% 93%



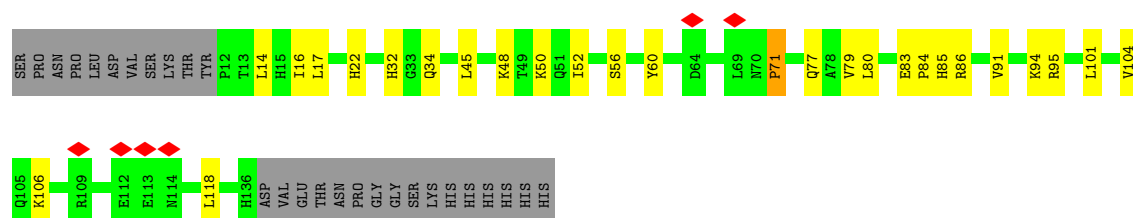
Chain AA: 56% 28% 16%



Chain BB: 74% 11% 14%



Chain CC: 64% 17% 18%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	120749	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; The contrast transfer function (CTF) was estimated per-image using CtfFind4. All further phase+amplitude correction was performed internally in Relion. Per-particle CTF refinement was done after polishing	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	54.4	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.011	Depositor
Minimum map value	-0.498	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	481.50003, 481.50003, 481.50003	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UR3, G7M, 8AN, 7MG, OMC, 5MC, 4SU, 1MG, OMU, 3TD, PSU, FME, 4OC, 2MA, H2U, 6MZ, 5MU, MA6, MG, 2MG, OMG, 0TD, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	B	0.49	0/2121	0.50	0/2852
2	C	0.45	0/1586	0.43	0/2134
3	D	0.41	0/1571	0.40	0/2113
4	E	0.32	0/1434	0.31	0/1926
5	F	0.28	0/1333	0.28	0/1805
6	G	0.21	0/1122	0.33	0/1515
7	H	0.13	0/993	0.40	0/1340
8	I	0.10	0/998	0.30	0/1348
9	J	0.45	0/1152	0.40	0/1551
10	K	0.44	0/955	0.42	0/1279
11	L	0.42	0/1062	0.45	0/1413
12	M	0.43	0/1093	0.37	0/1460
13	N	0.49	0/964	0.44	0/1289
14	O	0.35	0/902	0.31	0/1209
15	P	0.46	0/929	0.37	0/1242
16	Q	0.50	0/960	0.42	0/1278
17	R	0.43	0/829	0.36	0/1107
18	S	0.48	0/864	0.42	0/1156
19	T	0.41	0/752	0.35	0/1005
20	U	0.39	0/796	0.39	0/1062
21	V	0.37	0/766	0.36	0/1025
22	W	0.46	0/589	0.46	0/779
23	X	0.43	0/635	0.40	0/848
24	Y	0.34	0/502	0.30	0/667
25	Z	0.42	0/452	0.39	0/605
26	1	0.60	1/69286 (0.0%)	0.42	1/108087 (0.0%)
27	2	0.51	0/36588	0.35	0/57066
28	3	0.45	0/2872	0.30	0/4478
29	5	0.38	0/1672	0.34	0/2603
30	a	0.23	0/531	0.30	0/709
31	b	0.43	0/450	0.45	0/599

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	c	0.38	0/433	0.36	0/576
33	d	0.51	0/380	0.48	0/498
34	e	0.49	0/513	0.44	0/676
35	f	0.43	0/303	0.37	0/397
36	g	0.27	0/1791	0.29	0/2413
37	h	0.36	0/1663	0.35	0/2241
38	i	0.38	0/1665	0.31	0/2227
39	j	0.40	0/1165	0.42	0/1568
40	k	0.33	0/867	0.31	0/1171
41	l	0.30	0/1195	0.30	0/1602
42	m	0.41	0/989	0.37	0/1326
43	n	0.35	0/1034	0.34	0/1375
44	o	0.36	1/800 (0.1%)	0.41	0/1082
45	p	0.37	0/893	0.36	0/1205
46	q	0.42	0/960	0.38	0/1286
47	r	0.34	0/909	0.34	0/1215
48	s	0.37	0/817	0.32	0/1088
49	t	0.38	0/722	0.30	0/964
50	u	0.42	0/659	0.36	0/884
51	v	0.36	0/657	0.38	0/881
52	w	0.41	0/553	0.34	0/743
53	x	0.32	0/680	0.32	0/915
54	y	0.38	0/675	0.31	0/895
55	z	0.31	0/597	0.33	0/792
56	XX	0.50	0/197	0.32	0/306
57	AA	0.26	0/1102	0.47	0/1498
57	BB	0.33	0/1146	0.54	0/1555
57	CC	0.20	0/1082	0.46	0/1469
All	All	0.52	2/161206 (0.0%)	0.39	1/240398 (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
6	G	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	o	53	ILE	C-N	-5.38	1.22	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1	2069	G7M	O3'-P	5.16	1.61	1.56

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1	512	G	O4'-C1'-N9	5.50	116.45	108.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	G	71	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	B	2082	0	2154	26	0
2	C	1565	0	1616	18	0
3	D	1552	0	1618	14	0
4	E	1410	0	1444	16	0
5	F	1313	0	1358	9	0
6	G	1111	0	1148	34	0
7	H	980	0	1013	55	0
8	I	984	0	1035	30	0
9	J	1129	0	1162	13	0
10	K	946	0	1023	12	0
11	L	1053	0	1129	11	0
12	M	1074	0	1157	11	0
13	N	951	0	994	5	0
14	O	892	0	923	6	0
15	P	917	0	962	10	0
16	Q	947	0	1019	9	0
17	R	816	0	839	11	0
18	S	857	0	922	15	0
19	T	746	0	811	13	0
20	U	788	0	844	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	V	753	0	780	6	0
22	W	582	0	599	6	0
23	X	625	0	652	3	0
24	Y	501	0	531	3	0
25	Z	448	0	488	6	0
26	1	62336	0	31370	341	0
27	2	32929	0	16590	190	0
28	3	2569	0	1301	10	0
29	5	1622	0	831	12	0
30	a	522	0	521	10	0
31	b	444	0	458	5	0
32	c	426	0	464	12	0
33	d	377	0	418	4	0
34	e	504	0	572	5	0
35	f	302	0	340	3	0
36	g	1760	0	1787	25	0
37	h	1636	0	1710	24	0
38	i	1643	0	1707	11	0
39	j	1152	0	1196	16	0
40	k	848	0	846	9	0
41	l	1181	0	1238	23	0
42	m	979	0	1031	12	0
43	n	1022	0	1070	18	0
44	o	790	0	831	19	0
45	p	877	0	887	16	0
46	q	957	0	1017	7	0
47	r	900	0	965	10	0
48	s	805	0	844	10	0
49	t	714	0	734	11	0
50	u	649	0	666	6	0
51	v	648	0	691	4	0
52	w	544	0	560	4	0
53	x	663	0	688	13	0
54	y	669	0	719	3	0
55	z	589	0	629	11	0
56	XX	176	0	87	0	0
57	AA	1067	0	1045	31	0
57	BB	1111	0	1096	12	0
57	CC	1048	0	1030	17	0
58	1	290	0	0	0	0
58	2	128	0	0	0	0
58	3	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	5	3	0	0	0	0
58	B	1	0	0	0	0
58	BB	1	0	0	0	0
58	C	1	0	0	0	0
58	M	1	0	0	0	0
58	N	1	0	0	0	0
58	Q	1	0	0	0	0
58	b	1	0	0	0	0
58	i	1	0	0	0	0
59	5	10	0	10	1	0
60	a	1	0	0	0	0
60	f	1	0	0	0	0
61	B	2	0	0	0	0
All	All	149932	0	102170	1111	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 5.

All (1111) 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)
26:1:881:G:H1	26:1:895:U:H3	1.18	0.92
57:BB:77:GLN:HE21	57:BB:95:ARG:HA	1.40	0.86
26:1:2796:U:H3	26:1:2799:A:H61	1.21	0.85
27:2:69:G:H1	27:2:98:A:H61	1.25	0.85
27:2:75:G:O6	27:2:95:C:N4	2.11	0.84
7:H:107:GLU:HG2	7:H:109:LYS:H	1.42	0.83
27:2:1191:A:OP1	37:h:4:LYS:NZ	2.12	0.82
27:2:841:C:H2'	27:2:843:U:H5'	1.61	0.82
27:2:664:G:H22	27:2:741:G:H1	1.27	0.82
27:2:1057:G:O2'	37:h:188:GLU:OE1	1.97	0.81
27:2:1305:G:H21	27:2:1332:A:H2	1.27	0.81
16:Q:49:ASP:OD2	26:1:534:U:O2'	1.99	0.81
27:2:94:G:N1	27:2:97:G:O6	2.14	0.80
26:1:2069:G7M:N2	26:1:2442:C:O2	2.12	0.80
27:2:76:G:H1	27:2:93:U:H3	1.26	0.79
7:H:30:SER:O	26:1:1106:G:N2	2.15	0.79
10:K:38:ILE:HD11	10:K:112:PHE:HZ	1.48	0.79
27:2:1124:G:O2'	27:2:1145:A:N6	2.14	0.79
40:k:2:ARG:NH1	40:k:68:GLN:OE1	2.18	0.76
14:O:31:THR:HG22	14:O:33:ARG:H	1.48	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:k:1:MET:SD	40:k:1:MET:N	2.58	0.76
26:1:1869:G:N2	26:1:1871:A:O2'	2.17	0.76
57:AA:16:ILE:HD12	57:AA:29:ILE:HD12	1.67	0.76
18:S:4:ILE:HG13	18:S:106:VAL:HG22	1.67	0.75
26:1:2102:G:N1	26:1:2188:U:O2	2.15	0.75
27:2:1026:G:N1	27:2:1035:A:N1	2.35	0.74
57:AA:90:ASP:HB3	57:AA:102:PRO:HB3	1.69	0.73
7:H:56:ARG:HB2	26:1:1106:G:H4'	1.70	0.73
26:1:1169:A:H62	26:1:1180:U:H3	1.35	0.73
32:c:25:LYS:NZ	32:c:30:LYS:O	2.22	0.72
27:2:108:G:H5'	27:2:109:A:H5''	1.70	0.72
41:l:113:ASP:OD2	41:l:122:ASN:ND2	2.22	0.72
8:I:92:PRO:HB2	8:I:136:GLY:HA3	1.71	0.72
26:1:1056:G:H22	26:1:1102:C:H3'	1.54	0.72
2:C:141:ARG:NH2	26:1:1998:A:OP2	2.21	0.72
3:D:111:GLU:OE1	3:D:114:ARG:NH1	2.22	0.72
8:I:132:ALA:HB1	8:I:137:LEU:HB2	1.72	0.72
7:H:24:SER:OG	7:H:86:MET:SD	2.48	0.72
7:H:34:THR:HA	7:H:37:LYS:HD2	1.70	0.71
3:D:21:ARG:O	3:D:114:ARG:NH2	2.24	0.71
26:1:1085:A:O2'	26:1:1104:C:O2	2.09	0.71
57:AA:44:VAL:H	57:AA:63:MET:HE2	1.55	0.70
26:1:544:C:N4	26:1:549:G:O6	2.15	0.70
26:1:2114:A:N6	26:1:2119:A:N7	2.40	0.70
29:5:4:G:N2	29:5:68:C:O2	2.20	0.70
53:x:50:ALA:HB1	53:x:57:HIS:HB3	1.74	0.69
27:2:1297:G:O2'	41:l:114:LYS:NZ	2.24	0.69
26:1:1064:C:N4	26:1:1069:A:O2'	2.26	0.69
26:1:125:A:OP2	33:d:19:ARG:NH1	2.25	0.69
27:2:279:A:H5''	27:2:280:C:H3'	1.74	0.69
7:H:118:ILE:HG23	7:H:119:PRO:HD3	1.75	0.68
27:2:1137:C:O2	27:2:1138:G:N1	2.25	0.68
16:Q:92:ARG:NH1	26:1:1153:C:OP1	2.27	0.68
14:O:45:SER:OG	28:3:9:G:O2'	2.11	0.68
47:r:11:ASP:HA	47:r:45:ILE:HB	1.75	0.68
29:5:32:4OC:HM22	29:5:33:U:H5'	1.75	0.68
1:B:156:ARG:NH1	26:1:1818:U:OP2	2.27	0.68
6:G:97:ARG:HB3	6:G:112:LYS:HE3	1.76	0.67
7:H:31:ARG:HA	26:1:1054:A:H1'	1.77	0.67
27:2:998:C:O2	27:2:1043:G:N2	2.23	0.67
44:o:7:ARG:NH1	44:o:75:ASP:OD2	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:2:1004:A:OP1	27:2:1024:G:N1	2.27	0.67
12:M:66:ARG:NH1	12:M:104:GLU:OE2	2.27	0.67
6:G:132:PHE:HB2	6:G:140:ALA:HB3	1.76	0.67
6:G:96:THR:HG23	6:G:115:VAL:HB	1.76	0.67
7:H:100:ALA:O	7:H:103:ASN:ND2	2.29	0.67
17:R:83:TYR:CE1	26:1:1187:G:H5''	2.29	0.66
26:1:1064:C:N3	26:1:1074:G:N2	2.41	0.66
2:C:151:THR:HG22	26:1:2032:G:H21	1.60	0.66
27:2:203:G:O2'	27:2:465:A:N1	2.27	0.66
7:H:60:LEU:HD11	7:H:79:PRO:HG3	1.77	0.66
41:l:27:VAL:HG12	41:l:43:VAL:HG21	1.77	0.66
9:J:96:ARG:NH2	26:1:2640:G:OP1	2.28	0.66
42:m:9:ASP:OD2	42:m:13:ARG:NH1	2.29	0.66
14:O:45:SER:HG	28:3:9:G:HO2'	1.42	0.66
27:2:310:G:H5''	50:u:31:ARG:HB2	1.78	0.66
27:2:464:U:N3	27:2:467:U:OP2	2.27	0.66
41:l:40:GLU:OE2	43:n:41:ARG:NH1	2.29	0.66
41:l:68:ASN:ND2	41:l:130:ASN:OD1	2.28	0.66
57:CC:83:GLU:OE1	57:CC:86:ARG:N	2.29	0.66
27:2:769:G:H4'	27:2:1513:A:H4'	1.78	0.65
5:F:104:ASN:ND2	5:F:114:ASP:OD1	2.30	0.65
12:M:82:MET:HA	12:M:82:MET:HE2	1.77	0.65
27:2:83:C:O2'	27:2:86:G:O6	2.14	0.65
37:h:14:ILE:HG22	37:h:15:VAL:HG13	1.78	0.65
24:Y:11:VAL:O	24:Y:15:ASN:ND2	2.29	0.65
27:2:82:G:H1	27:2:86:G:H22	1.43	0.65
7:H:33:VAL:HA	26:1:1055:G:H4'	1.79	0.64
27:2:928:G:O2'	27:2:1533:C:OP1	2.14	0.64
7:H:42:ARG:NH1	26:1:1082:U:OP1	2.30	0.64
47:r:4:ILE:HD13	47:r:9:ILE:HD12	1.80	0.64
5:F:16:ASP:HB3	5:F:27:LYS:HB2	1.80	0.64
26:1:2857:G:N2	26:1:2860:A:OP2	2.21	0.64
5:F:172:LYS:NZ	26:1:2530:A:N7	2.46	0.64
7:H:23:LEU:H	7:H:23:LEU:HD23	1.63	0.64
26:1:1417:C:HO2'	26:1:1587:G:HO2'	1.38	0.64
26:1:1969:A:O2'	26:1:1972:G:N3	2.29	0.64
37:h:72:ARG:HB3	37:h:75:ILE:HD13	1.79	0.64
43:n:84:THR:HG23	43:n:98:LEU:HD13	1.81	0.64
57:AA:16:ILE:HB	57:AA:78:ALA:HB3	1.79	0.64
26:1:1064:C:H42	26:1:1074:G:H1	1.46	0.63
2:C:56:LYS:HB2	2:C:59:ARG:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:2:1008:U:N3	27:2:1021:A:N1	2.46	0.63
41:l:111:ARG:NH1	41:l:123:GLU:OE1	2.32	0.63
27:2:1152:A:OP1	44:o:70:HIS:ND1	2.30	0.63
57:BB:119:TYR:CE2	57:BB:133:LEU:HD11	2.34	0.63
57:CC:77:GLN:NE2	57:CC:94:LYS:O	2.25	0.63
26:1:138:U:O2'	26:1:141:G:O6	2.15	0.63
27:2:1007:U:OP1	48:s:19:LYS:NZ	2.32	0.63
43:n:123:ARG:NH1	43:n:124:ARG:O	2.28	0.63
15:P:89:ARG:NH1	15:P:113:ARG:O	2.31	0.63
26:1:355:U:H2'	26:1:356:G:H8	1.64	0.63
39:j:13:GLU:HG2	39:j:39:VAL:HG12	1.79	0.63
27:2:75:G:N1	27:2:95:C:N3	2.46	0.62
18:S:25:ARG:NH1	18:S:74:ILE:O	2.32	0.62
27:2:823:C:HO2'	42:m:2:SER:N	1.97	0.62
26:1:2131:U:H5'	26:1:2132:U:H5''	1.81	0.62
8:I:61:TYR:O	8:I:64:ARG:NH2	2.32	0.62
41:l:93:PRO:HA	41:l:96:ARG:HD3	1.81	0.62
44:o:82:LYS:NZ	44:o:82:LYS:O	2.28	0.62
36:g:5:SER:HB2	36:g:7:ARG:HH21	1.64	0.62
37:h:36:ASP:OD1	37:h:59:ARG:NH1	2.32	0.62
49:t:26:GLU:HG3	49:t:81:LEU:HD22	1.82	0.62
1:B:258:ARG:NH2	26:1:1800:C:OP1	2.33	0.62
6:G:51:ARG:HG2	6:G:55:GLU:HG2	1.81	0.62
8:I:101:SER:HB3	8:I:104:GLN:HB2	1.82	0.62
26:1:548:G:H3'	26:1:549:G:O4'	1.99	0.62
26:1:882:G:N2	26:1:895:U:O4'	2.33	0.62
41:l:111:ARG:NH2	41:l:126:ASP:OD2	2.33	0.62
5:F:89:LEU:HD23	5:F:94:TYR:HB3	1.82	0.62
19:T:1:MET:SD	26:1:139:U:N3	2.73	0.62
27:2:1527:U:OP2	55:z:42:THR:HG22	2.00	0.62
12:M:123:LYS:NZ	26:1:2483:C:N3	2.46	0.61
20:U:48:PRO:HG3	20:U:56:GLY:HA3	1.82	0.61
17:R:34:GLU:HG3	17:R:60:LYS:HD2	1.81	0.61
12:M:20:LEU:HD13	21:V:81:PRO:HG2	1.83	0.61
26:1:1056:G:O2'	26:1:1086:A:O2'	2.16	0.61
8:I:124:MET:SD	8:I:124:MET:N	2.74	0.61
57:CC:56:SER:O	57:CC:106:LYS:NZ	2.22	0.61
16:Q:76:TYR:OH	16:Q:92:ARG:NH1	2.34	0.61
26:1:1645:G:H5''	26:1:1646:C:H5'	1.83	0.61
27:2:562:U:H1'	46:q:12:ARG:HB3	1.82	0.61
57:CC:83:GLU:HG2	57:CC:84:PRO:HD2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:1527:G:N1	26:1:1544:A:OP2	2.31	0.61
30:a:13:THR:HG22	30:a:23:LYS:HG2	1.81	0.61
6:G:97:ARG:HH21	6:G:112:LYS:HD3	1.65	0.60
26:1:1047:G:HO2'	26:1:1110:G:H1	1.46	0.60
27:2:496:A:N3	27:2:496:A:H2'	2.16	0.60
13:N:24:MET:HE1	13:N:40:LYS:HD2	1.83	0.60
26:1:1478:G:H1	26:1:1513:U:H3	1.49	0.60
8:I:135:MET:HE2	26:1:1063:G:H1'	1.84	0.60
18:S:25:ARG:HG3	18:S:74:ILE:HG22	1.83	0.60
27:2:409:U:OP1	38:i:23:SER:OG	2.14	0.60
37:h:155:GLY:HA2	37:h:163:ALA:HB1	1.83	0.60
9:J:125:TYR:HH	9:J:132:HIS:HE2	1.45	0.60
27:2:890:G:O2'	27:2:906:A:N6	2.34	0.60
7:H:53:ARG:HD2	7:H:54:VAL:H	1.67	0.60
32:c:38:LYS:HB2	32:c:49:TYR:CD1	2.36	0.60
22:W:10:THR:OG1	22:W:11:ARG:N	2.35	0.60
26:1:1056:G:O2'	26:1:1103:A:N6	2.34	0.60
26:1:1779:U:H5	26:1:1784:A:N7	1.99	0.60
27:2:1346:A:OP1	43:n:122:ARG:NH1	2.31	0.60
26:1:1311:G:H21	26:1:1603:A:H62	1.50	0.60
45:p:126:LYS:NZ	45:p:127:ARG:H	2.00	0.60
3:D:188:MET:HE3	3:D:193:VAL:HG22	1.83	0.59
7:H:31:ARG:CZ	26:1:1053:C:H2'	2.32	0.59
4:E:122:PHE:HB3	4:E:163:ASP:OD1	2.02	0.59
26:1:1054:A:H2'	26:1:1055:G:H8	1.67	0.59
45:p:67:ALA:HB2	45:p:96:THR:HG23	1.84	0.59
57:AA:89:MET:SD	57:AA:89:MET:N	2.75	0.59
1:B:155:ALA:HB2	1:B:162:VAL:HG23	1.85	0.59
26:1:1871:A:O2'	26:1:1872:A:N7	2.35	0.59
53:x:36:ARG:NH2	53:x:75:ALA:O	2.36	0.59
57:AA:97:ARG:HD3	57:AA:99:PHE:CE2	2.37	0.59
3:D:46:GLN:O	3:D:88:ARG:NH2	2.35	0.59
26:1:1173:U:H4'	26:1:1174:U:H5'	1.84	0.59
26:1:2249:U:H3'	26:1:2250:G:H5''	1.84	0.59
27:2:842:U:H4'	27:2:846:G:C6	2.38	0.59
45:p:126:LYS:HZ1	45:p:127:ARG:H	1.50	0.59
46:q:55:VAL:HG21	46:q:80:ILE:HD11	1.85	0.59
4:E:131:GLY:HA2	4:E:153:ASP:HA	1.85	0.59
27:2:275:G:H5'	51:v:16:LYS:HE3	1.85	0.59
22:W:65:GLY:HA2	22:W:85:GLU:HB2	1.83	0.59
41:l:129:GLU:OE2	41:l:131:LYS:NZ	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:n:128:SER:OG	43:n:130:ARG:OXT	2.19	0.59
57:AA:83:GLU:OE1	57:AA:86:ARG:HG2	2.02	0.59
57:CC:14:LEU:HD23	57:CC:118:LEU:HD23	1.84	0.59
47:r:33:ILE:HD11	47:r:63:PHE:HE2	1.68	0.58
57:CC:32:HIS:O	57:CC:34:GLN:NE2	2.36	0.58
27:2:1103:C:OP1	36:g:95:ARG:NH2	2.36	0.58
7:H:6:GLN:O	7:H:9:GLN:NE2	2.36	0.58
26:1:1939:5MU:OP1	26:1:2604:U:O2'	2.20	0.58
27:2:107:G:O6	54:y:10:ARG:HD2	2.03	0.58
41:l:56:LYS:HG3	41:l:61:ALA:HB2	1.85	0.58
53:x:19:VAL:HG21	53:x:44:MET:HG2	1.85	0.58
29:5:19:G:OP1	29:5:60:U:N3	2.37	0.58
8:I:52:LEU:HD12	8:I:73:PRO:HG3	1.85	0.58
43:n:6:TYR:HB2	43:n:21:ILE:HG12	1.86	0.58
3:D:171:ASP:OD1	3:D:172:ALA:N	2.36	0.58
37:h:186:THR:HG22	37:h:199:LYS:HG2	1.85	0.58
6:G:114:GLU:N	6:G:114:GLU:OE1	2.36	0.58
27:2:376:G:H5''	50:u:5:ARG:HB2	1.86	0.58
20:U:86:ARG:NH2	20:U:100:SER:OG	2.36	0.58
39:j:70:ASN:O	39:j:70:ASN:ND2	2.37	0.58
9:J:114:LEU:HG	9:J:118:MET:HE3	1.84	0.57
12:M:18:ARG:HG2	28:3:90:C:H5''	1.86	0.57
39:j:105:ILE:O	39:j:112:ARG:NH2	2.36	0.57
44:o:8:ILE:HB	44:o:74:VAL:HG13	1.86	0.57
6:G:60:GLU:N	6:G:60:GLU:OE1	2.37	0.57
27:2:816:A:OP1	27:2:1526:G:O2'	2.20	0.57
7:H:40:GLU:OE2	7:H:101:LYS:NZ	2.35	0.57
26:1:2162:G:OP2	26:1:2164:C:N4	2.33	0.57
11:L:57:LEU:HD12	11:L:60:ARG:HD2	1.86	0.57
44:o:31:ARG:HG3	44:o:32:THR:N	2.19	0.57
27:2:1071:C:H2'	27:2:1072:G:H8	1.69	0.57
37:h:85:GLU:OE1	37:h:89:LYS:NZ	2.38	0.57
54:y:43:ASP:OD1	54:y:43:ASP:N	2.38	0.57
3:D:57:LYS:NZ	3:D:58:LYS:O	2.37	0.57
26:1:819:A:OP2	26:1:1187:G:N2	2.28	0.57
26:1:1537:G:C5	26:1:1538:G:H1'	2.39	0.57
1:B:107:PRO:HD2	1:B:110:LEU:HD22	1.86	0.57
27:2:1013:G:N2	27:2:1016:A:OP2	2.28	0.57
50:u:4:ILE:HG12	50:u:21:VAL:HG22	1.87	0.57
57:CC:45:LEU:HD22	57:CC:50:LYS:HE2	1.86	0.57
1:B:133:ARG:HB3	1:B:186:ALA:HB1	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:82:ARG:NH2	26:1:301:G:OP2	2.38	0.56
4:E:46:ASP:OD1	4:E:47:LYS:N	2.38	0.56
21:V:2:PHE:HB2	21:V:61:LEU:HD22	1.87	0.56
27:2:1218:C:H2'	27:2:1219:A:C8	2.41	0.56
27:2:1320:C:O2	53:x:36:ARG:NH1	2.37	0.56
48:s:23:LYS:HD2	48:s:51:LEU:HD21	1.88	0.56
7:H:72:LEU:HB3	7:H:73:LYS:HE2	1.88	0.56
57:BB:28:ARG:HG2	57:BB:38:GLU:OE1	2.05	0.56
7:H:31:ARG:NH1	26:1:1054:A:O4'	2.39	0.56
26:1:2101:A:H2'	26:1:2102:G:C8	2.41	0.56
26:1:2698:U:H2'	26:1:2699:C:C6	2.40	0.56
27:2:677:U:H3	27:2:713:G:H22	1.54	0.56
7:H:53:ARG:HD2	7:H:54:VAL:N	2.21	0.56
26:1:2162:G:O2'	26:1:2163:A:N7	2.38	0.56
10:K:58:LEU:HD11	10:K:86:LEU:HD13	1.88	0.56
7:H:11:ILE:HD11	7:H:66:GLY:H	1.71	0.56
7:H:42:ARG:HD3	8:I:119:ALA:H	1.70	0.56
26:1:2134:A:N6	26:1:2157:G:O2'	2.39	0.56
39:j:111:MET:HE2	39:j:125:ALA:HB1	1.88	0.56
27:2:933:G:O6	41:l:3:ARG:NH2	2.29	0.56
29:5:15:C:H5'	29:5:16:C:H5''	1.86	0.56
29:5:21:A:O2'	29:5:46:A:N6	2.39	0.56
8:I:133:ARG:O	26:1:1077:A:O2'	2.24	0.55
26:1:1414:C:N4	26:1:1415:U:O4	2.38	0.55
39:j:13:GLU:OE2	39:j:68:ARG:NH1	2.39	0.55
27:2:976:G:OP2	27:2:1358:U:O2'	2.25	0.55
26:1:1536:C:H4'	26:1:1537:G:H5''	1.87	0.55
7:H:107:GLU:HG2	7:H:109:LYS:N	2.19	0.55
1:B:136:PRO:O	1:B:139:SER:OG	2.25	0.55
6:G:137:GLU:N	6:G:137:GLU:OE1	2.39	0.55
11:L:85:VAL:HB	11:L:94:THR:HG22	1.89	0.55
20:U:39:ILE:HG13	20:U:40:ASN:H	1.72	0.55
24:Y:2:LYS:NZ	24:Y:5:GLU:OE1	2.40	0.55
26:1:84:A:N1	26:1:98:G:O2'	2.39	0.55
26:1:1796:U:H2'	26:1:1797:G:C8	2.42	0.55
8:I:117:THR:O	8:I:117:THR:OG1	2.21	0.55
27:2:395:C:OP1	57:BB:100[A]:ARG:NH2	2.39	0.55
27:2:1026:G:O6	27:2:1035:A:N6	2.40	0.55
1:B:75:PRO:HG2	1:B:97:LYS:HG3	1.89	0.55
2:C:151:THR:HG22	26:1:2032:G:N2	2.21	0.55
7:H:41:LEU:HD22	26:1:1083:U:H4'	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:281:C:H2'	26:1:282:A:H8	1.71	0.55
26:1:2792:A:H2	26:1:2805:C:N3	2.04	0.55
26:1:651:G:H5'	34:e:19:LYS:HG3	1.88	0.55
38:i:100:ASN:OD1	38:i:111:ARG:NH1	2.39	0.55
7:H:34:THR:N	26:1:1055:G:O2'	2.40	0.55
26:1:1102:C:H2'	26:1:1103:A:H8	1.72	0.55
49:t:47:LYS:H	49:t:47:LYS:HD2	1.71	0.55
1:B:165:VAL:HG21	1:B:181:MET:HE1	1.89	0.54
6:G:97:ARG:HH22	26:1:2220:U:H5''	1.71	0.54
27:2:67:C:H2'	27:2:68:G:C8	2.42	0.54
40:k:43:GLY:HA2	40:k:58:HIS:CE1	2.42	0.54
26:1:2116:G:N1	26:1:2162:G:OP2	2.39	0.54
40:k:3:HIS:NE2	40:k:65:GLU:OE2	2.41	0.54
55:z:62:ARG:NH1	55:z:63:GLU:OE1	2.41	0.54
26:1:645:C:H2'	26:1:647:G:C8	2.42	0.54
26:1:2273:A:H2'	26:1:2274:A:C8	2.43	0.54
27:2:412:A:H62	27:2:431:A:H61	1.54	0.54
27:2:485:U:H5'	57:AA:48:LYS:HE2	1.89	0.54
55:z:66:ARG:HH11	55:z:67:ARG:HH11	1.55	0.54
12:M:17:ASN:OD1	12:M:97:GLN:NE2	2.36	0.54
12:M:31:PHE:HD1	12:M:132:THR:HG22	1.72	0.54
27:2:82:G:H22	27:2:84:U:H6	1.55	0.54
57:BB:83:GLU:HB3	57:BB:84:PRO:HD2	1.89	0.54
26:1:476:G:N1	26:1:479:A:OP2	2.36	0.54
42:m:11:LEU:HD22	42:m:75:ILE:HD11	1.89	0.54
27:2:564:C:OP1	46:q:12:ARG:HD2	2.08	0.54
27:2:1174:G:H2'	27:2:1175:G:H5'	1.90	0.54
44:o:42:LEU:HB2	44:o:71:LEU:HB3	1.89	0.54
26:1:2297:A:N1	26:1:2321:U:H5	2.05	0.54
27:2:579:A:H2'	27:2:580:C:C6	2.42	0.54
36:g:165:ASP:HB3	36:g:168:HIS:HB3	1.90	0.54
57:CC:50:LYS:HE3	57:CC:60:TYR:CE2	2.42	0.54
26:1:1028:A:N6	26:1:1125:G:H2'	2.23	0.54
57:AA:44:VAL:N	57:AA:63:MET:HE2	2.23	0.54
26:1:720:U:H2'	26:1:721:A:C8	2.43	0.53
27:2:74:A:HO2'	27:2:75:G:H8	1.56	0.53
19:T:5:GLU:OE1	19:T:5:GLU:N	2.42	0.53
26:1:1264:A:OP1	31:b:16:ARG:NH2	2.41	0.53
27:2:662:U:O2'	27:2:836:G:OP1	2.26	0.53
49:t:26:GLU:N	49:t:26:GLU:OE1	2.41	0.53
7:H:11:ILE:HD11	7:H:66:GLY:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:b:29:SER:OG	31:b:40:ARG:NH1	2.41	0.53
2:C:13:ARG:HH21	15:P:56:HIS:HA	1.74	0.53
7:H:42:ARG:HD2	26:1:1082:U:H5''	1.90	0.53
26:1:1172:C:O2'	26:1:1173:U:O4'	2.20	0.53
26:1:2792:A:C2	26:1:2793:C:N3	2.76	0.53
27:2:754:C:O5'	49:t:72:ARG:NH2	2.42	0.53
27:2:1516:2MG:N2	27:2:1519:MA6:OP2	2.40	0.53
2:C:133:THR:CG2	26:1:1993:U:H4'	2.38	0.53
26:1:1045:C:O2	26:1:1047:G:N1	2.42	0.53
26:1:1064:C:N4	26:1:1070:A:OP2	2.41	0.53
32:c:10:LYS:HD2	32:c:54:ILE:HA	1.91	0.53
37:h:70:THR:HG21	37:h:76:VAL:HG21	1.91	0.53
18:S:73:LYS:HB2	18:S:106:VAL:HB	1.92	0.52
26:1:355:U:H2'	26:1:356:G:C8	2.45	0.52
26:1:2114:A:H62	26:1:2169:A:N6	2.07	0.52
26:1:832:U:H2'	26:1:833:A:C8	2.44	0.52
26:1:1796:U:H2'	26:1:1797:G:H8	1.75	0.52
4:E:69:LYS:HG2	4:E:84:PRO:HA	1.90	0.52
27:2:1266:G:N2	27:2:1269:A:OP2	2.39	0.52
41:l:79:ARG:HA	41:l:84:THR:HA	1.91	0.52
14:O:61:GLN:OE1	14:O:61:GLN:N	2.43	0.52
26:1:580:U:H2'	26:1:581:C:C6	2.44	0.52
26:1:1932:A:H2'	26:1:1933:G:O4'	2.09	0.52
20:U:81:ASP:OD2	20:U:98:SER:OG	2.27	0.52
26:1:250:G:H2'	26:1:251:A:C8	2.45	0.52
26:1:1076:C:H2'	26:1:1077:A:C8	2.44	0.52
27:2:1347:G:O6	43:n:12:ARG:NH2	2.42	0.52
38:i:172:GLU:HB2	38:i:183:LYS:HZ1	1.74	0.52
27:2:946:A:H2'	27:2:947:G:C8	2.44	0.52
8:I:122:GLU:OE1	8:I:122:GLU:N	2.37	0.52
25:Z:6:LYS:NZ	25:Z:37:GLU:OE1	2.33	0.52
27:2:1332:A:H2'	27:2:1333:A:O4'	2.09	0.52
7:H:95:LEU:HD23	7:H:98:GLU:HG3	1.90	0.52
7:H:102:ALA:HA	7:H:105:LYS:HB3	1.91	0.52
15:P:62:ARG:NH1	15:P:71:GLU:OE2	2.42	0.52
27:2:127:G:O3'	51:v:6:ARG:NH2	2.43	0.52
27:2:842:U:H3'	27:2:843:U:H5''	1.92	0.52
27:2:1225:A:H2'	27:2:1226:C:C5	2.45	0.52
6:G:109:GLU:CD	6:G:109:GLU:H	2.18	0.52
27:2:374:A:H5''	27:2:452:A:C2	2.45	0.52
26:1:2134:A:O2'	26:1:2159:G:N3	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:2477:U:O2	35:f:4:ARG:NH2	2.41	0.51
45:p:15:GLN:NE2	45:p:76:GLU:O	2.40	0.51
55:z:64:ASN:OD1	55:z:65:ALA:N	2.42	0.51
9:J:78:THR:HB	26:1:2641:G:H5''	1.93	0.51
26:1:2130:U:O2'	26:1:2158:A:N1	2.43	0.51
26:1:2291:U:OP1	26:1:2380:C:O2'	2.24	0.51
8:I:38:CYS:HA	8:I:41:PHE:HB2	1.92	0.51
27:2:126:G:OP1	27:2:605:U:O2'	2.25	0.51
45:p:94:GLU:H	45:p:94:GLU:CD	2.18	0.51
18:S:12:SER:O	18:S:101:SER:OG	2.22	0.51
26:1:1059:G:H2'	26:1:1060:U:C5	2.46	0.51
26:1:1508:A:H4'	26:1:1509:A:H5'	1.93	0.51
27:2:75:G:H2'	27:2:76:G:H8	1.76	0.51
27:2:1277:C:O2'	27:2:1279:G:H8	1.93	0.51
50:u:9:HIS:O	50:u:16:PHE:HB3	2.10	0.51
57:AA:37:ALA:HB2	57:AA:135:ILE:HD13	1.92	0.51
2:C:59:ARG:HH12	26:1:2830:C:H3'	1.75	0.51
26:1:2151:U:H2'	26:1:2152:G:C8	2.45	0.51
36:g:73:LYS:C	36:g:75:ALA:H	2.19	0.51
27:2:97:G:C2	27:2:98:A:H1'	2.46	0.51
42:m:87:LYS:HB2	42:m:125:ILE:HD11	1.93	0.51
43:n:55:VAL:HG11	43:n:94:LEU:HD22	1.93	0.51
6:G:98:ASP:HA	6:G:101:ASP:HB2	1.93	0.51
15:P:88:ARG:NH2	15:P:110:ILE:O	2.33	0.51
16:Q:4:VAL:HG22	26:1:1199:U:H1'	1.92	0.51
26:1:885:C:O2	26:1:891:G:N1	2.40	0.51
26:1:2328:A:H2'	26:1:2329:U:C6	2.46	0.51
27:2:160:A:H2'	27:2:161:A:O4'	2.11	0.51
12:M:111:GLU:CD	12:M:111:GLU:H	2.18	0.51
27:2:1532:U:O4	27:2:1533:C:N4	2.43	0.51
15:P:52:ASN:O	26:1:2845:U:H5''	2.10	0.51
26:1:586:A:N1	26:1:809:G:O2'	2.37	0.51
26:1:1548:A:H2'	26:1:1549:A:C8	2.46	0.51
43:n:28:ILE:HG12	43:n:63:LEU:HD23	1.93	0.51
1:B:182:ARG:NH2	26:1:1800:C:OP2	2.41	0.51
26:1:887:A:O2'	26:1:889:C:OP2	2.20	0.51
26:1:1183:U:H2'	26:1:1184:U:C6	2.46	0.51
6:G:93:SER:HB3	6:G:123:ARG:HG2	1.93	0.50
8:I:33:ASN:OD1	8:I:36:GLU:N	2.44	0.50
27:2:1391:U:H2'	27:2:1392:G:C8	2.47	0.50
57:AA:97:ARG:HB2	57:AA:100:ARG:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:64:TRP:HB2	12:M:104:GLU:HB2	1.93	0.50
26:1:878:A:H3'	26:1:879:G:H8	1.75	0.50
26:1:910:A:N3	26:1:2264:C:O2'	2.41	0.50
51:v:25:ILE:HB	51:v:42:THR:HB	1.94	0.50
1:B:161:TYR:HB3	1:B:194:GLU:HG2	1.93	0.50
3:D:189:THR:HG22	3:D:191:ASP:H	1.76	0.50
21:V:60:VAL:HG22	21:V:73:LYS:HE3	1.93	0.50
27:2:1071:C:H2'	27:2:1072:G:C8	2.47	0.50
55:z:58:LYS:NZ	55:z:59:LYS:HG3	2.27	0.50
19:T:94:ASP:OD1	19:T:94:ASP:N	2.41	0.50
26:1:723:C:H2'	26:1:724:U:O4'	2.11	0.50
27:2:501:C:H2'	27:2:502:A:C8	2.47	0.50
32:c:6:ARG:HG2	32:c:24:THR:HB	1.93	0.50
43:n:25:ASN:OD1	43:n:25:ASN:N	2.44	0.50
7:H:34:THR:HG21	26:1:1057:A:H1'	1.93	0.50
26:1:614:A:O2'	26:1:615:U:OP2	2.25	0.50
27:2:1323:G:H2'	27:2:1324:A:C8	2.47	0.50
27:2:1356:G:H2'	27:2:1357:A:C8	2.47	0.50
1:B:36:LYS:NZ	1:B:38:SER:HB2	2.26	0.50
7:H:15:VAL:HG21	7:H:66:GLY:HA3	1.93	0.50
18:S:55:ILE:HG23	18:S:66:ILE:HD12	1.94	0.50
26:1:1913:A:N1	27:2:1492:A:O2'	2.42	0.50
27:2:1299:A:O2'	27:2:1300:G:H4'	2.12	0.50
48:s:10:GLU:HG3	48:s:63:ARG:HD2	1.94	0.50
27:2:1412:C:H2'	27:2:1413:A:C8	2.46	0.50
42:m:38:ASN:O	42:m:42:GLU:HG2	2.11	0.50
57:CC:17:LEU:HD23	57:CC:77:GLN:HG3	1.93	0.50
2:C:181:ASP:HB3	2:C:186:LEU:HB2	1.93	0.50
8:I:88:GLY:HA3	26:1:1063:G:O2'	2.12	0.50
26:1:1386:C:H2'	26:1:1387:A:C8	2.47	0.50
36:g:61:ALA:HB2	36:g:221:VAL:HG23	1.94	0.50
37:h:6:HIS:CE1	37:h:8:ASN:HB3	2.47	0.50
1:B:51:THR:HG21	26:1:1814:G:H4'	1.93	0.49
22:W:70:GLU:HG3	22:W:72:LYS:HD3	1.93	0.49
27:2:736:C:OP1	52:w:61:ARG:NH1	2.40	0.49
2:C:56:LYS:HE3	26:1:2830:C:H5''	1.93	0.49
26:1:743:A:O2'	26:1:1659:G:OP1	2.30	0.49
27:2:97:G:H2'	27:2:98:A:O4'	2.12	0.49
57:AA:63:MET:HE3	57:AA:63:MET:HA	1.94	0.49
26:1:1:G:H2'	26:1:2:G:H8	1.77	0.49
26:1:1054:A:H2'	26:1:1055:G:C8	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:1070:A:N7	26:1:1096:A:O2'	2.39	0.49
27:2:672:U:H2'	27:2:673:A:C8	2.46	0.49
40:k:37:HIS:HB3	40:k:97:THR:HG22	1.94	0.49
57:AA:12:PRO:HB2	57:AA:82:ALA:HB3	1.95	0.49
7:H:92:ALA:HB1	7:H:129:LEU:HB3	1.94	0.49
20:U:8:ASP:OD1	20:U:8:ASP:N	2.45	0.49
26:1:612:G:H2'	26:1:614:A:C8	2.48	0.49
26:1:753:A:H2'	26:1:754:U:C6	2.47	0.49
36:g:57:LEU:HD13	36:g:217:VAL:HG23	1.94	0.49
6:G:66:ASN:ND2	6:G:138:VAL:HG21	2.28	0.49
21:V:55:GLU:OE1	21:V:55:GLU:N	2.37	0.49
25:Z:3:LYS:HD3	25:Z:4:THR:H	1.78	0.49
30:a:44:PHE:HD1	30:a:45:THR:HG23	1.78	0.49
53:x:35:SER:OG	53:x:38:SER:OG	2.23	0.49
55:z:7:ARG:N	55:z:10:GLU:OE1	2.46	0.49
9:J:109:LEU:O	9:J:111:LYS:NZ	2.40	0.49
26:1:2183:A:H2'	26:1:2184:A:H8	1.78	0.49
27:2:79:G:H2'	27:2:80:A:C8	2.48	0.49
34:e:14:PHE:O	34:e:15:LYS:HD2	2.13	0.49
45:p:13:ARG:NE	45:p:76:GLU:OE2	2.33	0.49
17:R:29:THR:O	17:R:29:THR:OG1	2.30	0.49
10:K:38:ILE:HD11	10:K:112:PHE:CZ	2.38	0.49
57:AA:20:PHE:HB2	57:AA:74:SER:OG	2.12	0.49
6:G:8:LYS:NZ	6:G:9:VAL:O	2.39	0.49
7:H:23:LEU:HA	7:H:118:ILE:HG21	1.95	0.49
26:1:1066:U:H2'	26:1:1067:A:H2'	1.94	0.49
26:1:1563:U:H2'	26:1:1564:C:C6	2.48	0.49
27:2:568:G:O6	46:q:2:ALA:HB2	2.13	0.49
57:CC:22:HIS:CE1	57:CC:71:PRO:HB3	2.47	0.49
27:2:683:G:N2	45:p:39:GLY:O	2.46	0.49
1:B:199:GLU:CD	1:B:199:GLU:H	2.21	0.48
4:E:108:VAL:HG11	4:E:176:PRO:HG2	1.95	0.48
8:I:112:LYS:HB3	8:I:115:ASP:HB3	1.94	0.48
10:K:76:VAL:HG13	15:P:73:VAL:HB	1.95	0.48
13:N:56:LYS:NZ	13:N:90:ARG:O	2.46	0.48
15:P:33:VAL:HG22	15:P:38:LYS:HG3	1.94	0.48
28:3:1:U:O2'	28:3:2:G:H8	1.96	0.48
52:w:10:PHE:HB2	52:w:12:ARG:NH2	2.28	0.48
6:G:43:ASN:HA	6:G:46:PHE:HB3	1.94	0.48
26:1:197:A:N6	26:1:2430:A:H2'	2.28	0.48
27:2:6:G:O2'	27:2:7:A:H8	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:2:432:A:H4'	57:CC:48:LYS:CE	2.44	0.48
36:g:6:MET:H	36:g:7:ARG:NH2	2.11	0.48
55:z:31:GLU:HA	55:z:34:ARG:HG2	1.95	0.48
57:AA:30:PHE:CE1	57:AA:35:LEU:HG	2.48	0.48
9:J:134:ALA:O	26:1:2898:U:O2'	2.26	0.48
26:1:2591:C:H2'	26:1:2592:G:C8	2.48	0.48
36:g:188:ASP:HB2	36:g:204:ASP:OD2	2.14	0.48
39:j:156:LYS:HG2	42:m:71:VAL:HG13	1.95	0.48
45:p:36:ASP:OD2	45:p:40:ASN:HB2	2.13	0.48
20:U:8:ASP:HB2	20:U:24:LYS:HE3	1.94	0.48
27:2:74:A:C8	27:2:75:G:N7	2.82	0.48
44:o:26:VAL:O	44:o:30:LYS:HG2	2.13	0.48
2:C:133:THR:HG22	26:1:1993:U:H4'	1.94	0.48
8:I:21:PRO:HB2	8:I:22:PRO:HD3	1.96	0.48
18:S:6:LYS:HB2	26:1:494:G:H4'	1.96	0.48
29:5:18:G:H8	29:5:18:G:OP1	1.96	0.48
42:m:96:MET:HE3	42:m:99:LEU:HB2	1.96	0.48
18:S:49:LYS:NZ	26:1:488:G:O2'	2.35	0.48
26:1:2469:A:N6	26:1:2481:G:O2'	2.44	0.48
27:2:1040:U:H2'	27:2:1041:G:C8	2.48	0.48
16:Q:68:ALA:O	16:Q:72:ASN:ND2	2.46	0.48
26:1:1176:U:H4'	26:1:1177:G:O4'	2.13	0.48
27:2:1040:U:H2'	27:2:1041:G:H8	1.79	0.48
29:5:63:G:H2'	29:5:64:G:H8	1.78	0.48
40:k:2:ARG:HE	40:k:91:ARG:NH1	2.11	0.48
9:J:37:ARG:NH1	26:1:1007:C:OP1	2.45	0.48
14:O:4:LYS:NZ	28:3:7:G:OP1	2.42	0.48
17:R:81:LYS:HD2	26:1:973:A:H5''	1.95	0.48
27:2:79:G:H1	27:2:90:C:H42	1.62	0.48
49:t:21:ASP:O	49:t:22:THR:HG22	2.13	0.48
6:G:135:HIS:ND1	6:G:137:GLU:OE1	2.47	0.48
27:2:978:A:O2'	27:2:1322:C:H5	1.97	0.48
43:n:47:VAL:HG13	43:n:80:ARG:HD3	1.96	0.48
26:1:1590:A:H2'	26:1:1591:A:C8	2.48	0.48
26:1:2189:U:O2'	26:1:2190:G:H5''	2.14	0.48
26:1:2343:U:O2'	26:1:2373:G:O2'	2.24	0.48
11:L:82:LEU:HD22	11:L:90:VAL:HG21	1.96	0.47
18:S:97:LEU:HD12	18:S:97:LEU:HA	1.75	0.47
26:1:281:C:H2'	26:1:282:A:C8	2.49	0.47
44:o:52:LEU:HD23	44:o:62:ARG:HG2	1.95	0.47
4:E:17:MET:HE2	4:E:25:VAL:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:48:ASN:ND2	5:F:48:ASN:O	2.47	0.47
19:T:53:VAL:HG11	19:T:87:LEU:HD13	1.96	0.47
37:h:79:LYS:HD3	37:h:80:LYS:N	2.29	0.47
6:G:68:ARG:O	6:G:72:ILE:N	2.47	0.47
8:I:135:MET:HE1	26:1:1062:G:N3	2.29	0.47
26:1:2554:U:H2'	26:1:2555:U:C6	2.49	0.47
30:a:30:HIS:ND1	30:a:31:ASP:O	2.45	0.47
37:h:45:LYS:HB3	37:h:45:LYS:HE2	1.76	0.47
45:p:58:SER:O	45:p:91:PRO:HG2	2.14	0.47
18:S:93:ALA:HB2	26:1:1614:A:C2	2.50	0.47
26:1:1:G:H2'	26:1:2:G:C8	2.50	0.47
26:1:753:A:H2'	26:1:754:U:H6	1.79	0.47
26:1:1141:U:H4'	26:1:1142:A:O4'	2.14	0.47
26:1:2146:C:O2'	26:1:2147:A:O5'	2.26	0.47
36:g:118:GLU:O	36:g:122:GLN:HG2	2.15	0.47
51:v:78:VAL:HG11	51:v:81:LYS:HE2	1.97	0.47
54:y:25:ARG:O	54:y:29:ARG:HG3	2.14	0.47
24:Y:7:ARG:NH2	26:1:78:U:OP1	2.48	0.47
25:Z:44:ILE:HA	25:Z:47:MET:HE3	1.95	0.47
26:1:856:G:H2'	26:1:857:G:C8	2.49	0.47
27:2:750:C:H4'	49:t:21:ASP:HA	1.96	0.47
26:1:125:A:H2	33:d:9:VAL:HG12	1.78	0.47
26:1:1808:A:H3'	26:1:1809:A:C8	2.50	0.47
30:a:11:GLU:HG2	30:a:25:ARG:HG3	1.97	0.47
39:j:45:ARG:HA	39:j:72:ILE:O	2.14	0.47
50:u:61:VAL:HG22	50:u:67:ILE:HD11	1.96	0.47
2:C:156:PHE:CE1	9:J:81:ILE:HD13	2.50	0.47
7:H:39:THR:HG21	7:H:105:LYS:HD3	1.96	0.47
11:L:77:ILE:CD1	11:L:108:ALA:HB1	2.45	0.47
13:N:45:ARG:HG2	13:N:95:THR:HG21	1.97	0.47
27:2:1086:U:H3	27:2:1099:G:H22	1.63	0.47
27:2:1377:A:OP1	41:l:92:ARG:NH2	2.48	0.47
32:c:32:GLU:H	32:c:32:GLU:CD	2.23	0.47
48:s:46:LEU:HD22	53:x:13:LEU:HD23	1.96	0.47
6:G:72:ILE:HG23	6:G:108:VAL:HG22	1.96	0.47
8:I:135:MET:SD	26:1:1062:G:O2'	2.65	0.47
26:1:45:G:H5''	26:1:46:G:H5'	1.97	0.47
27:2:131:A:H2'	27:2:132:C:C6	2.50	0.47
27:2:1477:U:H2'	27:2:1478:U:C6	2.50	0.47
36:g:4:VAL:HG21	36:g:212:LEU:HD21	1.97	0.47
44:o:7:ARG:HD2	44:o:73:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:x:3:ARG:HH21	53:x:7:LYS:HD3	1.80	0.47
2:C:23:PRO:HB3	26:1:2682:A:C2	2.50	0.47
19:T:22:THR:HG23	19:T:26:LYS:HE3	1.97	0.47
27:2:492:C:H2'	27:2:493:A:C8	2.49	0.47
59:5:104:FME:HB3	59:5:104:FME:O1	2.15	0.47
37:h:152:GLU:HG3	37:h:167:TRP:HB3	1.96	0.47
4:E:147:ASP:OD1	4:E:147:ASP:N	2.48	0.47
7:H:97:LYS:HA	7:H:100:ALA:HB3	1.97	0.47
18:S:93:ALA:HB2	26:1:1614:A:H2	1.80	0.47
26:1:191:A:H2'	26:1:192:C:C6	2.49	0.47
26:1:475:C:O2	26:1:479:A:N6	2.40	0.47
26:1:1176:U:H5''	26:1:1177:G:O5'	2.14	0.47
26:1:1922:G:C2'	26:1:1923:U:H5'	2.45	0.47
26:1:2615:U:C2	31:b:4:GLN:HA	2.50	0.47
27:2:859:G:H2'	27:2:860:A:C8	2.50	0.47
44:o:30:LYS:HD3	44:o:36:VAL:HG12	1.97	0.47
45:p:14:LYS:NZ	45:p:15:GLN:O	2.45	0.47
45:p:97:ILE:HG22	55:z:12:PHE:HZ	1.80	0.47
2:C:33:ARG:HE	2:C:73:VAL:HG13	1.79	0.46
7:H:97:LYS:HZ3	7:H:125:ARG:HD2	1.81	0.46
26:1:1056:G:HO2'	26:1:1086:A:HO2'	1.58	0.46
26:1:1450:G:C6	26:1:1451:C:N4	2.82	0.46
26:1:1469:A:H2'	26:1:1470:A:C8	2.49	0.46
26:1:1682:G:H2'	26:1:1683:U:C6	2.50	0.46
26:1:2859:G:H2'	26:1:2860:A:C8	2.50	0.46
27:2:626:G:OP1	50:u:35:ARG:NH2	2.48	0.46
27:2:718:A:H5'	45:p:119:ASN:CG	2.41	0.46
3:D:2:GLU:HG3	3:D:11:ALA:HB1	1.97	0.46
17:R:31:GLU:N	17:R:31:GLU:OE1	2.48	0.46
43:n:118:LEU:HD22	43:n:124:ARG:HG3	1.98	0.46
2:C:46:ARG:NH2	2:C:88:GLU:O	2.47	0.46
19:T:53:VAL:HG13	19:T:91:GLN:HB3	1.98	0.46
20:U:33:LYS:HB3	20:U:64:ALA:HB1	1.97	0.46
25:Z:13:ALA:O	25:Z:21:LYS:HE2	2.15	0.46
39:j:88:VAL:HG22	39:j:93:ARG:HG2	1.96	0.46
57:BB:96:ILE:HG22	57:BB:98:PRO:HD3	1.95	0.46
6:G:17:ASP:OD1	6:G:17:ASP:N	2.49	0.46
8:I:123:ALA:HB1	26:1:1081:U:H4'	1.96	0.46
26:1:1870:C:H2'	26:1:1871:A:C5	2.51	0.46
26:1:2522:U:O2'	26:1:2647:U:OP1	2.22	0.46
27:2:1023:U:H2'	27:2:1024:G:O4'	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:m:50:LYS:HB3	42:m:50:LYS:HE3	1.58	0.46
42:m:105:SER:HB3	42:m:126:ILE:HD11	1.98	0.46
57:CC:16:ILE:HD11	57:CC:80:LEU:HD12	1.98	0.46
27:2:1145:A:O2'	27:2:1146:A:O5'	2.31	0.46
42:m:87:LYS:HG3	42:m:91:GLU:HB2	1.98	0.46
7:H:58:THR:HG23	7:H:63:ALA:HB3	1.96	0.46
13:N:38:LEU:HD11	13:N:42:LYS:HE3	1.98	0.46
20:U:41:LEU:HB3	20:U:60:GLU:OE1	2.16	0.46
27:2:3:A:H5''	27:2:4:U:O4'	2.16	0.46
27:2:860:A:H2'	27:2:861:G:O4'	2.16	0.46
37:h:111:LEU:HD22	37:h:146:ALA:HB2	1.97	0.46
26:1:752:A:H3'	33:d:1:MET:SD	2.56	0.46
26:1:2776:A:H4'	26:1:2777:G:H5''	1.97	0.46
27:2:821:G:H2'	27:2:822:U:C6	2.51	0.46
28:3:66:A:H61	28:3:107:G:H2'	1.80	0.46
1:B:246:THR:HG23	1:B:252:THR:HG22	1.98	0.46
6:G:68:ARG:HE	6:G:68:ARG:HB3	1.45	0.46
7:H:78:GLY:HA2	7:H:82:ILE:HD11	1.97	0.46
26:1:2291:U:H2'	26:1:2292:U:C6	2.50	0.46
27:2:108:G:H5'	27:2:109:A:C5'	2.44	0.46
27:2:202:G:HO2'	27:2:468:A:H8	1.61	0.46
27:2:932:C:H2'	27:2:933:G:C8	2.51	0.46
37:h:130:PHE:CE2	37:h:166:GLU:HG3	2.51	0.46
44:o:15:HIS:HB3	44:o:70:HIS:CE1	2.50	0.46
44:o:57:VAL:O	44:o:58:ASN:ND2	2.49	0.46
2:C:125:TRP:CG	2:C:160:LYS:HB3	2.50	0.46
8:I:92:PRO:HD2	26:1:1076:C:O2'	2.16	0.46
16:Q:9:ILE:HD13	16:Q:9:ILE:HA	1.79	0.46
23:X:59:ILE:HG12	23:X:67:VAL:HG21	1.97	0.46
39:j:165:LEU:HD13	42:m:114:ARG:NH1	2.31	0.46
49:t:21:ASP:OD1	49:t:22:THR:N	2.44	0.46
57:AA:97:ARG:HB2	57:AA:100:ARG:HG3	1.98	0.46
7:H:26:VAL:HG12	7:H:84:TYR:HA	1.98	0.46
26:1:545:U:O2'	26:1:546:U:H4'	2.16	0.46
27:2:17:U:H2'	27:2:18:C:C6	2.51	0.46
37:h:130:PHE:HE2	37:h:166:GLU:HG3	1.81	0.46
53:x:12:ASP:OD1	53:x:35:SER:OG	2.28	0.46
10:K:7:MET:HE3	10:K:7:MET:HB3	1.79	0.45
26:1:1703:G:H2'	26:1:1704:C:C6	2.51	0.45
27:2:673:A:H2'	27:2:674:G:C8	2.51	0.45
34:e:14:PHE:C	34:e:15:LYS:HD2	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:n:57:MET:HB3	43:n:61:LEU:HD23	1.98	0.45
5:F:154:PRO:HD3	5:F:162:VAL:O	2.17	0.45
10:K:78:ARG:NH2	26:1:2685:G:OP1	2.49	0.45
13:N:8:ARG:HH11	13:N:43:GLU:HG2	1.81	0.45
27:2:1530:G:O6	55:z:46:LYS:NZ	2.41	0.45
32:c:11:LEU:HD21	32:c:34:LEU:HD23	1.97	0.45
39:j:45:ARG:HH21	39:j:71:MET:HE3	1.81	0.45
39:j:111:MET:CE	39:j:125:ALA:HB1	2.46	0.45
41:l:5:ARG:HG2	41:l:7:ILE:HG23	1.99	0.45
2:C:125:TRP:CD1	2:C:160:LYS:HB3	2.50	0.45
26:1:1056:G:N2	26:1:1104:C:H41	2.14	0.45
37:h:156:ARG:H	37:h:163:ALA:HA	1.81	0.45
1:B:43:ARG:HA	1:B:48:ARG:O	2.17	0.45
10:K:1:MET:HG3	10:K:32:TYR:CD1	2.51	0.45
26:1:276:U:H1'	26:1:277:G:C8	2.52	0.45
27:2:575:G:O2'	27:2:821:G:OP2	2.31	0.45
27:2:1193:G:O6	37:h:3:GLN:NE2	2.49	0.45
27:2:1379:G:OP2	41:l:5:ARG:NH2	2.49	0.45
53:x:3:ARG:HH11	53:x:10:PHE:HB2	1.80	0.45
57:CC:77:GLN:O	57:CC:91:VAL:HA	2.16	0.45
1:B:29:PRO:HG2	1:B:34:LEU:HD11	1.98	0.45
5:F:47:ASP:OD1	5:F:47:ASP:N	2.50	0.45
6:G:3:VAL:CG1	6:G:36:ALA:HB1	2.47	0.45
7:H:35:VAL:HA	7:H:38:MET:HB2	1.97	0.45
7:H:81:LEU:HA	26:1:1107:G:H4'	1.98	0.45
41:l:139:GLU:O	41:l:143:ARG:N	2.49	0.45
43:n:24:GLY:HA3	43:n:62:ASP:OD2	2.16	0.45
57:AA:31:ARG:HH21	57:AA:115:VAL:HG21	1.81	0.45
26:1:1064:C:H41	26:1:1070:A:P	2.40	0.45
26:1:1405:U:H2'	26:1:1406:U:C6	2.51	0.45
26:1:1794:A:H2'	26:1:1795:C:C6	2.52	0.45
26:1:2127:G:O6	26:1:2160:C:N4	2.50	0.45
26:1:2791:G:N1	26:1:2792:A:N3	2.65	0.45
27:2:41:G:H2'	27:2:42:G:C8	2.52	0.45
27:2:209:U:H3'	27:2:210:C:O2	2.17	0.45
27:2:1273:C:H2'	27:2:1274:A:O4'	2.17	0.45
36:g:214:LEU:HA	36:g:217:VAL:HG12	1.99	0.45
38:i:148:LYS:HE2	38:i:148:LYS:HB3	1.82	0.45
40:k:88:MET:SD	40:k:90:MET:HE2	2.57	0.45
41:l:31:MET:HE2	41:l:36:LYS:HD3	1.97	0.45
48:s:3:LYS:HB2	48:s:6:MET:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:27:VAL:HG22	7:H:109:LYS:HE3	1.99	0.45
7:H:64:VAL:HA	7:H:67:THR:HB	1.99	0.45
19:T:68:LYS:O	19:T:74:ILE:HD12	2.17	0.45
26:1:714:U:H1'	26:1:717:C:H5	1.81	0.45
26:1:969:G:H2'	26:1:970:U:C6	2.52	0.45
26:1:1068:G:N2	26:1:1095:A:O3'	2.49	0.45
26:1:2014:A:H2'	26:1:2015:A:C8	2.52	0.45
26:1:2030:6MZ:C2	26:1:2499:C:H5''	2.46	0.45
26:1:2327:A:H2'	26:1:2328:A:C8	2.52	0.45
30:a:49:ARG:HA	30:a:49:ARG:HD2	1.71	0.45
46:q:110:ARG:HB3	46:q:119:VAL:HG21	1.99	0.45
3:D:57:LYS:HE2	3:D:57:LYS:HB2	1.77	0.45
7:H:126:LEU:HB3	7:H:129:LEU:HD11	1.99	0.45
19:T:3:ARG:HH12	26:1:144:A:H5'	1.81	0.45
23:X:3:ARG:O	23:X:12:PRO:HD3	2.16	0.45
26:1:2191:A:H2'	26:1:2192:U:C6	2.52	0.45
27:2:99:C:O2'	27:2:100:G:H8	1.99	0.45
27:2:977:A:O2'	27:2:979:C:OP2	2.33	0.45
27:2:1228:C:H1'	47:r:116:ILE:HD11	1.99	0.45
18:S:22:ASP:OD1	18:S:25:ARG:NH2	2.46	0.45
26:1:1061:U:O2'	26:1:1063:G:OP1	2.23	0.45
27:2:69:G:H1	27:2:98:A:N6	2.04	0.45
27:2:381:C:H2'	27:2:382:A:O4'	2.17	0.45
8:I:88:GLY:H	26:1:1064:C:H4'	1.82	0.45
26:1:479:A:N3	26:1:481:G:H5''	2.32	0.45
26:1:1070:A:O2'	26:1:1097:U:O3'	2.35	0.45
27:2:28:A:O2'	27:2:296:U:OP1	2.30	0.45
31:b:38:HIS:HB3	31:b:44:THR:HG22	1.99	0.45
26:1:1149:G:H2'	26:1:1150:C:C6	2.51	0.44
26:1:2251:OMG:H1'	26:1:2251:OMG:HM23	1.62	0.44
26:1:2896:C:H2'	26:1:2897:U:C6	2.52	0.44
27:2:468:A:H5''	27:2:469:C:H5	1.81	0.44
39:j:44:GLY:HA3	39:j:74:VAL:H	1.82	0.44
47:r:11:ASP:OD1	47:r:11:ASP:N	2.46	0.44
26:1:1104:C:H3'	26:1:1105:U:C6	2.53	0.44
26:1:2135:A:H62	26:1:2156:G:H21	1.66	0.44
27:2:524:G:H2'	27:2:525:C:C6	2.52	0.44
43:n:106:ARG:NH1	43:n:107:ASP:O	2.43	0.44
57:AA:23:ARG:HH12	57:AA:68:PRO:HG3	1.82	0.44
6:G:71:LYS:HD3	6:G:71:LYS:HA	1.76	0.44
7:H:8:LYS:HZ2	26:1:1046:A:N6	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:91:ASP:OD1	11:L:92:LEU:N	2.45	0.44
26:1:1542:U:H2'	26:1:1543:G:O4'	2.17	0.44
41:l:57:SER:HB3	41:l:60:GLU:HG2	2.00	0.44
6:G:117:LEU:HD23	6:G:122:LEU:HD13	2.00	0.44
7:H:101:LYS:HE3	7:H:101:LYS:HB3	1.80	0.44
26:1:1094:U:N3	26:1:1097:U:OP2	2.45	0.44
26:1:2159:G:N2	26:1:2160:C:N3	2.66	0.44
26:1:2183:A:H2'	26:1:2184:A:C8	2.53	0.44
26:1:2557:G:H2'	26:1:2558:C:C6	2.52	0.44
27:2:382:A:H2'	27:2:383:A:C8	2.52	0.44
27:2:1029:U:N3	27:2:1031:C:O2	2.50	0.44
27:2:1126:U:OP1	44:o:7:ARG:NH2	2.50	0.44
36:g:3:THR:OG1	36:g:4:VAL:N	2.47	0.44
38:i:197:GLU:OE1	38:i:197:GLU:N	2.33	0.44
15:P:53:ARG:NH2	26:1:2720:U:OP1	2.42	0.44
19:T:33:LYS:HE3	19:T:33:LYS:HB2	1.65	0.44
26:1:1059:G:OP2	26:1:1060:U:H3'	2.17	0.44
27:2:736:C:H2'	27:2:737:C:C6	2.53	0.44
30:a:33:ASN:HD21	47:r:50:GLU:HG2	1.83	0.44
57:AA:78:ALA:HA	57:AA:91:VAL:HG12	1.99	0.44
4:E:160:ALA:HB1	4:E:165:GLU:HB2	2.00	0.44
16:Q:76:TYR:CZ	16:Q:80:ILE:HG13	2.53	0.44
26:1:877:A:C6	26:1:899:A:C6	3.05	0.44
26:1:1589:U:O2'	26:1:1590:A:H8	2.01	0.44
26:1:2233:U:H2'	26:1:2234:G:C8	2.52	0.44
6:G:97:ARG:HE	6:G:112:LYS:HD3	1.83	0.44
26:1:1677:A:H2'	26:1:1678:A:C8	2.52	0.44
27:2:93:U:H2'	27:2:94:G:H4'	1.99	0.44
27:2:1106:G:H5''	37:h:172:ARG:HG2	2.00	0.44
37:h:51:SER:HB2	37:h:115:LEU:HD22	2.00	0.44
39:j:94:VAL:HG13	39:j:111:MET:HE3	2.00	0.44
57:BB:82:ALA:HB2	57:BB:118:LEU:HD13	1.99	0.44
7:H:34:THR:O	7:H:38:MET:N	2.50	0.44
7:H:53:ARG:CZ	7:H:55:VAL:HA	2.48	0.44
8:I:131:THR:OG1	26:1:1060:U:O4	2.24	0.44
26:1:936:A:H2'	26:1:937:C:C6	2.52	0.44
26:1:2187:U:H2'	26:1:2188:U:O4'	2.18	0.44
26:1:2502:G:H5''	26:1:2503:2MA:H5''	2.00	0.44
26:1:2700:A:H2'	26:1:2701:U:C6	2.53	0.44
27:2:1021:A:N3	27:2:1021:A:H2'	2.32	0.44
57:AA:102:PRO:HG2	57:AA:105:GLN:HE21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:ASN:OD1	1:B:23:GLU:HG2	2.18	0.44
26:1:1790:C:H2'	26:1:1791:A:C5	2.53	0.44
27:2:1140:C:HO2'	27:2:1141:C:C5'	2.31	0.44
28:3:106:G:H2'	28:3:107:G:O4'	2.18	0.44
39:j:81:LEU:HD11	39:j:96:MET:HB3	1.99	0.44
26:1:277:G:H4'	26:1:278:A:C4	2.53	0.43
26:1:1594:U:H2'	26:1:1595:C:C6	2.53	0.43
26:1:2834:G:H2'	26:1:2879:A:H61	1.83	0.43
27:2:208:U:O2'	27:2:211:G:O6	2.36	0.43
27:2:1031:C:O3'	27:2:1032:G:N2	2.51	0.43
29:5:63:G:H2'	29:5:64:G:C8	2.53	0.43
38:i:140:ASN:N	38:i:182:PHE:O	2.51	0.43
2:C:148:GLN:O	26:1:2052:A:H4'	2.18	0.43
8:I:36:GLU:OE2	8:I:39:LYS:NZ	2.38	0.43
26:1:1704:C:H2'	26:1:1705:A:C8	2.52	0.43
26:1:2086:U:H2'	26:1:2087:G:C8	2.53	0.43
38:i:170:TRP:CD2	38:i:186:PRO:HB3	2.52	0.43
55:z:66:ARG:NH1	55:z:67:ARG:HD3	2.34	0.43
57:AA:58:GLY:HA2	57:AA:126:TYR:CD1	2.53	0.43
57:AA:83:GLU:HG2	57:AA:84:PRO:HD2	2.00	0.43
6:G:12:LEU:HD22	6:G:19:VAL:HG21	2.00	0.43
6:G:97:ARG:HE	6:G:112:LYS:CD	2.31	0.43
10:K:109:SER:O	10:K:113:MET:HE2	2.18	0.43
11:L:141:LYS:HB3	11:L:141:LYS:HE2	1.81	0.43
21:V:14:LYS:HB2	28:3:98:G:H1	1.84	0.43
26:1:754:U:H2'	26:1:755:U:C6	2.53	0.43
43:n:88:MET:HE3	43:n:95:ARG:CZ	2.48	0.43
46:q:50:ARG:HG3	46:q:90:LEU:HD21	2.00	0.43
4:E:96:MET:HE2	4:E:96:MET:HB3	1.90	0.43
4:E:115:ARG:NH1	30:a:50:ASP:HB3	2.33	0.43
26:1:370:G:O2'	26:1:424:G:OP1	2.33	0.43
26:1:910:A:H2'	26:1:911:A:C8	2.53	0.43
26:1:1966:A:N3	26:1:2592:G:O2'	2.49	0.43
27:2:692:U:O2'	27:2:694:A:N7	2.41	0.43
36:g:219:ALA:O	36:g:223:GLU:HG2	2.19	0.43
37:h:155:GLY:O	37:h:196:ILE:HG12	2.18	0.43
38:i:192:SER:OG	38:i:194:ASP:OD2	2.36	0.43
44:o:5:ARG:HE	44:o:7:ARG:NH1	2.16	0.43
57:AA:22:HIS:CE1	57:AA:71:PRO:HB3	2.54	0.43
16:Q:105:ALA:HA	17:R:47:VAL:HG21	2.00	0.43
20:U:91:LYS:HE3	20:U:91:LYS:HB2	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:59:LEU:HD12	22:W:80:ILE:HD12	2.00	0.43
27:2:52:C:H2'	27:2:53:A:C8	2.54	0.43
36:g:68:LEU:HB3	36:g:161:LEU:HD12	2.00	0.43
26:1:278:A:H2	26:1:361:G:C2	2.36	0.43
26:1:1028:A:H2'	26:1:1029:A:C8	2.54	0.43
26:1:2590:A:H2'	26:1:2591:C:C6	2.54	0.43
27:2:78:A:H2'	27:2:79:G:C8	2.54	0.43
31:b:43:ILE:HG22	31:b:49:TYR:HB2	2.00	0.43
4:E:80:ARG:HB2	4:E:83:TYR:CE2	2.53	0.43
7:H:61:ARG:HH21	26:1:1046:A:P	2.41	0.43
18:S:89:ALA:HB1	26:1:748:G:C8	2.54	0.43
20:U:14:LEU:HD11	20:U:71:ALA:HB2	2.00	0.43
26:1:595:C:H2'	26:1:596:U:C6	2.54	0.43
26:1:2107:G:H3'	26:1:2108:A:H8	1.84	0.43
26:1:2788:C:H2'	26:1:2789:C:C6	2.53	0.43
27:2:842:U:H3'	27:2:843:U:C5'	2.49	0.43
48:s:63:ARG:NH1	48:s:68:GLY:O	2.48	0.43
55:z:41:PRO:HA	55:z:44:GLU:HG2	2.01	0.43
8:I:126:ARG:HB2	26:1:1080:A:H4'	2.00	0.43
19:T:67:VAL:CG1	19:T:74:ILE:HD11	2.49	0.43
27:2:451:A:H61	27:2:481:G:H5'	1.83	0.43
1:B:51:THR:HG23	1:B:54:ILE:HD12	2.01	0.43
8:I:32:VAL:HG22	8:I:64:ARG:HD3	2.01	0.43
26:1:1056:G:N2	26:1:1103:A:OP2	2.50	0.43
26:1:1175:A:OP1	26:1:1177:G:H1'	2.19	0.43
27:2:40:C:OP1	57:BB:100[B]:ARG:NH1	2.52	0.43
33:d:3:ARG:HA	33:d:3:ARG:HD3	1.77	0.43
1:B:241:GLY:HA3	26:1:2597:G:H5'	2.00	0.43
3:D:168:ASP:OD2	3:D:170:ARG:NH1	2.51	0.43
17:R:1:MET:HE3	17:R:101:ILE:HB	2.01	0.43
20:U:45:HIS:HD2	26:1:483:A:C8	2.37	0.43
26:1:784:G:H5'	26:1:785:G:OP1	2.19	0.43
26:1:1428:C:C5	26:1:1569:A:H5''	2.54	0.43
26:1:2329:U:H2'	26:1:2330:G:C8	2.54	0.43
29:5:23:C:H2'	29:5:24:U:C6	2.54	0.43
34:e:29:LEU:HD23	34:e:29:LEU:HA	1.90	0.43
42:m:43:GLU:HG3	42:m:101:ILE:HD13	2.01	0.43
4:E:42:GLU:HG3	4:E:49:LEU:HD13	2.00	0.42
4:E:62:GLY:HA3	4:E:95:ARG:HH21	1.84	0.42
12:M:55:ARG:HD2	26:1:2469:A:H4'	2.01	0.42
26:1:1778:U:H2'	26:1:1784:A:N6	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:2171:A:O2'	26:1:2173:A:OP1	2.36	0.42
27:2:131:A:O2'	27:2:262:A:N3	2.39	0.42
27:2:555:U:H2'	27:2:556:C:C6	2.54	0.42
44:o:17:LEU:HD21	44:o:93:ALA:HB3	2.00	0.42
45:p:30:THR:HG21	45:p:63:ALA:HB2	2.00	0.42
1:B:97:LYS:HE2	1:B:97:LYS:HB3	1.85	0.42
4:E:125:ARG:HA	4:E:125:ARG:HD3	1.80	0.42
6:G:48:GLU:HA	6:G:52:ALA:HB2	2.01	0.42
8:I:80:LYS:HE3	8:I:137:LEU:HD11	2.01	0.42
26:1:1047:G:O2'	26:1:1110:G:N1	2.44	0.42
26:1:2172:U:H4'	26:1:2174:C:OP2	2.19	0.42
27:2:1530:G:H2'	27:2:1531:A:C8	2.54	0.42
29:5:17:U:H4'	29:5:18:G:O5'	2.19	0.42
32:c:8:LYS:HA	32:c:24:THR:HA	2.00	0.42
45:p:60:PRO:HD3	45:p:91:PRO:HB3	2.01	0.42
46:q:74:LEU:HD12	46:q:74:LEU:HA	1.84	0.42
53:x:48:THR:HG22	53:x:61:PHE:HD1	1.84	0.42
21:V:23:ALA:O	21:V:25:LYS:HG3	2.19	0.42
26:1:1939:5MU:O2	26:1:1967:C:H4'	2.19	0.42
26:1:2455:G:H2'	26:1:2456:C:C6	2.54	0.42
27:2:399:G:H2'	27:2:400:C:C6	2.54	0.42
29:5:58:A:O2'	29:5:60:U:OP2	2.25	0.42
43:n:97:GLU:HA	43:n:100:LYS:HE2	2.01	0.42
47:r:33:ILE:HD11	47:r:63:PHE:CE2	2.51	0.42
57:AA:118:LEU:O	57:AA:121:VAL:HG12	2.18	0.42
57:CC:48:LYS:O	57:CC:52:ILE:HG12	2.20	0.42
5:F:155:GLU:HG3	5:F:157:TYR:H	1.84	0.42
11:L:77:ILE:HD11	11:L:108:ALA:HB1	2.00	0.42
26:1:283:G:H2'	26:1:284:U:O4'	2.20	0.42
26:1:632:A:H2'	26:1:633:A:C8	2.54	0.42
26:1:2114:A:C8	26:1:2167:U:H4'	2.54	0.42
26:1:2246:G:H2'	26:1:2247:A:C8	2.54	0.42
27:2:667:G:H4'	49:t:51:HIS:ND1	2.34	0.42
36:g:187:VAL:HG13	36:g:191:SER:HB2	2.01	0.42
39:j:161:VAL:O	39:j:165:LEU:N	2.42	0.42
1:B:180:GLU:OE2	26:1:1799:G:O2'	2.34	0.42
7:H:43:LYS:HZ2	7:H:95:LEU:HD22	1.85	0.42
11:L:64:PHE:CZ	34:e:15:LYS:HD3	2.54	0.42
17:R:88:GLY:O	26:1:1224:U:H4'	2.19	0.42
23:X:30:LEU:HD12	26:1:2230:G:H5''	2.02	0.42
26:1:549:G:H2'	26:1:550:C:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:642:U:O2'	26:1:644:A:N7	2.41	0.42
26:1:1197:G:H2'	26:1:1198:U:C6	2.55	0.42
26:1:1744:A:H3'	26:1:1745:A:H8	1.85	0.42
26:1:2037:A:H2'	26:1:2038:G:C8	2.55	0.42
26:1:2514:U:H2'	26:1:2515:C:C6	2.54	0.42
27:2:74:A:O2'	27:2:75:G:H8	2.03	0.42
27:2:337:G:H2'	27:2:338:A:C8	2.55	0.42
27:2:518:C:H4'	27:2:519:C:H5''	2.02	0.42
27:2:737:C:H2'	27:2:738:C:C6	2.55	0.42
27:2:1417:G:N2	27:2:1482:G:H2'	2.34	0.42
30:a:18:CYS:HB2	30:a:40:CYS:HB3	2.01	0.42
47:r:16:VAL:HG13	47:r:34:LEU:HD12	2.01	0.42
49:t:67:LEU:HD12	49:t:67:LEU:HA	1.85	0.42
57:AA:16:ILE:HD12	57:AA:29:ILE:CD1	2.45	0.42
7:H:4:ASN:O	7:H:8:LYS:N	2.53	0.42
12:M:102:LEU:HD11	12:M:126:ILE:HD11	2.01	0.42
26:1:139:U:O2	26:1:139:U:H2'	2.19	0.42
26:1:634:C:H2'	26:1:635:C:C6	2.54	0.42
27:2:1479:C:H2'	27:2:1480:A:C8	2.54	0.42
53:x:3:ARG:NH1	53:x:10:PHE:HB2	2.35	0.42
57:AA:112:GLU:CD	57:AA:117:GLY:HA3	2.44	0.42
57:CC:94:LYS:C	57:CC:95:ARG:HG3	2.45	0.42
6:G:57:LYS:HA	6:G:57:LYS:HD3	1.88	0.42
7:H:33:VAL:HG13	26:1:1055:G:H4'	2.01	0.42
7:H:97:LYS:HD2	7:H:100:ALA:HB3	2.02	0.42
14:O:83:LEU:HD11	14:O:114:GLY:HA3	2.02	0.42
19:T:48:GLN:HA	19:T:53:VAL:O	2.19	0.42
20:U:34:VAL:HG13	20:U:67:VAL:HG22	2.00	0.42
26:1:760:G:H2'	26:1:761:A:O4'	2.19	0.42
26:1:1073:A:H2'	26:1:1074:G:O4'	2.19	0.42
27:2:460:A:H2'	27:2:461:A:C8	2.54	0.42
45:p:72:ASP:N	45:p:72:ASP:OD1	2.52	0.42
26:1:1534:U:N3	26:1:1536:C:O2	2.52	0.42
26:1:1999:C:H5''	26:1:2723:C:O2'	2.20	0.42
26:1:2190:G:H2'	26:1:2191:A:H8	1.85	0.42
5:F:11:VAL:HG23	5:F:15:VAL:HB	2.02	0.42
7:H:31:ARG:HD3	26:1:1054:A:C4'	2.50	0.42
9:J:30:THR:HG21	26:1:1005:C:O2'	2.19	0.42
10:K:8:LEU:HD22	10:K:84:CYS:HB3	2.02	0.42
20:U:43:LYS:O	26:1:480:A:O2'	2.38	0.42
26:1:288:U:H2'	26:1:289:G:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:742:A:H2'	26:1:743:A:C8	2.55	0.42
26:1:1060:U:N1	26:1:1062:G:H5'	2.35	0.42
26:1:2547:A:H2'	26:1:2548:U:C6	2.55	0.42
26:1:2636:C:H2'	26:1:2637:U:C6	2.55	0.42
27:2:246:A:N1	27:2:278:G:O2'	2.40	0.42
27:2:1024:G:H2'	27:2:1025:U:C6	2.54	0.42
36:g:54:LEU:HD22	36:g:220:THR:HG21	2.01	0.42
44:o:81:GLU:HA	44:o:84:VAL:HG12	2.01	0.42
1:B:36:LYS:HZ3	1:B:38:SER:HB2	1.85	0.42
6:G:62:LEU:HD23	6:G:62:LEU:HA	1.92	0.42
9:J:7:LYS:HE2	26:1:538:A:H5''	2.02	0.42
10:K:23:LYS:HB2	10:K:23:LYS:HE2	1.82	0.42
17:R:48:LYS:HE2	17:R:103:ALA:HB1	2.02	0.42
26:1:1668:A:O2'	26:1:1674:G:N7	2.50	0.42
27:2:692:U:H1'	27:2:695:A:N7	2.33	0.42
27:2:1060:U:OP1	48:s:85:ARG:NH2	2.44	0.42
32:c:11:LEU:HB3	32:c:49:TYR:HB3	2.02	0.42
1:B:240:PHE:CD2	1:B:240:PHE:O	2.73	0.41
10:K:70:ARG:NH2	26:1:2727:A:O2'	2.53	0.41
26:1:56:A:H2'	26:1:57:C:O4'	2.19	0.41
26:1:1266:G:O2'	26:1:2012:G:O6	2.33	0.41
27:2:1305:G:HO2'	27:2:1306:A:H8	1.63	0.41
57:AA:97:ARG:HD3	57:AA:99:PHE:CZ	2.55	0.41
2:C:59:ARG:NH1	26:1:2830:C:H3'	2.35	0.41
11:L:144:GLU:N	11:L:144:GLU:OE1	2.53	0.41
15:P:91:ALA:HB3	15:P:111:LYS:HG3	2.01	0.41
22:W:72:LYS:HB3	22:W:72:LYS:HE2	1.84	0.41
26:1:12:U:H2'	26:1:12:U:O2	2.20	0.41
26:1:739:A:H1'	26:1:740:C:H5	1.85	0.41
26:1:1637:A:H5'	26:1:1760:C:O2'	2.20	0.41
26:1:1722:A:N6	26:1:1738:G:H1'	2.34	0.41
27:2:789:U:O2'	27:2:791:G:N7	2.52	0.41
27:2:842:U:O2'	27:2:845:A:OP2	2.33	0.41
38:i:188:ARG:NH1	38:i:192:SER:O	2.35	0.41
41:l:76:LYS:HE2	41:l:89:VAL:HG11	2.02	0.41
44:o:85:ASP:O	44:o:89:ARG:HG2	2.21	0.41
3:D:41:GLN:HG2	3:D:43:THR:HG23	2.01	0.41
6:G:86:ASP:C	6:G:87:GLU:HG3	2.44	0.41
16:Q:15:LYS:HB3	16:Q:15:LYS:HE2	1.83	0.41
25:Z:54:MET:HE3	25:Z:54:MET:HB2	1.88	0.41
26:1:1177:G:HO2'	26:1:1178:C:H6	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1:1534:U:H4'	26:1:1535:A:H2	1.84	0.41
26:1:1681:G:N3	26:1:1762:A:H2'	2.35	0.41
27:2:99:C:O2'	27:2:100:G:H5'	2.20	0.41
27:2:1279:G:O2'	27:2:1281:C:OP2	2.28	0.41
48:s:52:PRO:O	48:s:55:SER:OG	2.28	0.41
1:B:13:ARG:HD3	26:1:728:G:H4'	2.03	0.41
19:T:33:LYS:HG3	19:T:80:TRP:CE3	2.55	0.41
22:W:12:ASN:ND2	26:1:2278:A:OP2	2.44	0.41
27:2:52:C:H2'	27:2:53:A:H8	1.85	0.41
27:2:68:G:C6	27:2:69:G:H1'	2.55	0.41
41:l:36:LYS:HG2	43:n:41:ARG:HH22	1.85	0.41
47:r:34:LEU:HD13	47:r:41:GLU:HA	2.02	0.41
49:t:44:ALA:O	49:t:47:LYS:HE3	2.21	0.41
53:x:21:LYS:O	53:x:25:SER:OG	2.35	0.41
6:G:9:VAL:HG23	6:G:12:LEU:HB2	2.01	0.41
6:G:42:LYS:HB3	6:G:42:LYS:HE2	1.76	0.41
11:L:63:LYS:HE2	26:1:2394:C:H5''	2.02	0.41
18:S:59:GLU:CD	18:S:66:ILE:HD11	2.45	0.41
26:1:666:A:H2'	26:1:667:U:C6	2.55	0.41
26:1:2526:G:O2'	35:f:34:LYS:NZ	2.46	0.41
27:2:714:G:H2'	27:2:715:A:C8	2.56	0.41
27:2:1171:A:H2'	27:2:1172:C:C6	2.56	0.41
27:2:1299:A:N3	27:2:1299:A:H2'	2.35	0.41
32:c:8:LYS:HD3	32:c:54:ILE:HD13	2.03	0.41
32:c:23:THR:OG1	32:c:24:THR:N	2.54	0.41
35:f:2:LYS:HE2	35:f:32:LYS:O	2.20	0.41
36:g:3:THR:OG1	36:g:51:ASN:OD1	2.36	0.41
36:g:124:GLY:O	36:g:128:LYS:HD2	2.20	0.41
36:g:174:LYS:HB3	36:g:174:LYS:NZ	2.35	0.41
57:CC:83:GLU:CD	57:CC:85:HIS:H	2.28	0.41
7:H:94:ARG:HD2	7:H:95:LEU:HG	2.02	0.41
17:R:55:ASP:OD1	17:R:55:ASP:N	2.54	0.41
25:Z:3:LYS:HD3	25:Z:4:THR:N	2.35	0.41
26:1:645:C:H2'	26:1:647:G:N7	2.36	0.41
26:1:1671:U:O2'	26:1:1673:G:N7	2.50	0.41
26:1:1736:U:H2'	26:1:1737:G:O4'	2.20	0.41
26:1:2098:U:H2'	26:1:2099:U:O4'	2.20	0.41
27:2:608:A:H2'	27:2:609:A:O4'	2.21	0.41
36:g:20:THR:HA	36:g:39:HIS:CE1	2.55	0.41
44:o:30:LYS:HA	44:o:30:LYS:HD2	1.92	0.41
1:B:225:MET:HE2	26:1:782:A:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:114:GLU:CD	7:H:116:GLU:H	2.28	0.41
8:I:91:LYS:HE2	26:1:1076:C:H5''	2.02	0.41
9:J:74:TYR:O	9:J:86:GLN:HA	2.21	0.41
18:S:59:GLU:OE1	18:S:66:ILE:HD11	2.21	0.41
27:2:202:G:O2'	27:2:468:A:H8	2.04	0.41
52:w:12:ARG:HA	52:w:12:ARG:HD3	1.60	0.41
4:E:148:ARG:HB3	4:E:150:ARG:NH1	2.36	0.41
20:U:51:ALA:O	20:U:52:LEU:HB2	2.20	0.41
26:1:361:G:O2'	26:1:362:A:H8	2.04	0.41
26:1:1028:A:H61	26:1:1125:G:H2'	1.85	0.41
26:1:1055:G:H1	26:1:1104:C:N4	2.19	0.41
26:1:1846:G:C6	26:1:1847:A:C6	3.09	0.41
26:1:2800:A:C2	26:1:2895:G:H1'	2.54	0.41
27:2:658:C:H1'	49:t:22:THR:HG21	2.01	0.41
27:2:1145:A:HO2'	27:2:1146:A:P	2.43	0.41
36:g:157:LEU:HD13	36:g:179:LEU:HD13	2.02	0.41
6:G:83:LYS:HB3	6:G:83:LYS:HE3	1.71	0.41
8:I:71:LYS:HE2	8:I:71:LYS:HB3	1.96	0.41
8:I:107:GLU:O	8:I:110:GLN:HG2	2.21	0.41
11:L:78:ARG:HG2	11:L:113:ALA:HB3	2.02	0.41
26:1:373:U:H2'	26:1:374:A:H8	1.86	0.41
26:1:643:A:N1	26:1:2369:A:O2'	2.51	0.41
26:1:948:C:H1'	26:1:984:A:C8	2.56	0.41
26:1:1083:U:O2'	26:1:1085:A:OP2	2.24	0.41
26:1:1106:G:H2'	26:1:1107:G:C8	2.55	0.41
26:1:2358:A:H2'	26:1:2359:C:O4'	2.20	0.41
26:1:2646:C:H2'	26:1:2647:U:O4'	2.20	0.41
27:2:75:G:N2	27:2:96:U:C2	2.89	0.41
27:2:452:A:H62	27:2:480:U:H3	1.67	0.41
27:2:918:A:H2'	27:2:919:A:O4'	2.21	0.41
27:2:1255:G:O2'	27:2:1258:G:N3	2.50	0.41
27:2:1402:4OC:H6	27:2:1402:4OC:O5'	2.21	0.41
28:3:112:G:H2'	28:3:113:C:C6	2.56	0.41
32:c:50:LYS:HE2	32:c:50:LYS:HB2	1.80	0.41
36:g:71:GLY:O	36:g:93:ASN:HA	2.21	0.41
37:h:12:LEU:HD23	37:h:12:LEU:HA	1.91	0.41
38:i:41:HIS:HB3	38:i:44:ARG:HD3	2.03	0.41
38:i:151:LYS:HE2	38:i:151:LYS:HB3	1.94	0.41
40:k:67:PRO:HG2	40:k:70:VAL:HG23	2.03	0.41
41:l:72:THR:HG23	41:l:96:ARG:HH22	1.86	0.41
44:o:37:ARG:NE	44:o:37:ARG:HA	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:w:26:ILE:HD13	52:w:26:ILE:HA	1.90	0.41
57:AA:43:VAL:HG13	57:AA:63:MET:HE1	2.03	0.41
1:B:145:GLU:HG2	1:B:151:GLY:C	2.46	0.41
9:J:96:ARG:HD2	9:J:99:ARG:HG2	2.03	0.41
19:T:65:GLY:N	19:T:79:ASP:OD1	2.42	0.41
26:1:576:U:H2'	26:1:577:G:C8	2.56	0.41
26:1:1102:C:H2'	26:1:1103:A:C8	2.55	0.41
36:g:8:ASP:OD1	36:g:8:ASP:N	2.50	0.41
40:k:9:MET:SD	40:k:86:ARG:HB3	2.61	0.41
48:s:16:LEU:HD12	48:s:54:ASP:HB2	2.02	0.41
53:x:20:GLU:O	53:x:24:GLU:HG3	2.21	0.41
57:BB:60:TYR:HA	57:BB:61:PRO:HD3	1.93	0.41
26:1:1802:A:H2'	26:1:1803:A:C8	2.55	0.40
27:2:717:U:H4'	45:p:119:ASN:HD22	1.86	0.40
27:2:721:G:H4'	27:2:722:G:O4'	2.22	0.40
27:2:1463:U:H2'	27:2:1464:U:C6	2.56	0.40
37:h:86:LYS:HE3	37:h:86:LYS:HB2	1.78	0.40
39:j:56:VAL:HB	39:j:57:PRO:HD3	2.03	0.40
48:s:38:ASP:OD1	48:s:39:GLU:N	2.54	0.40
57:AA:92:TYR:HD2	57:AA:100:ARG:HB3	1.86	0.40
57:AA:119:TYR:CZ	57:AA:133:LEU:HD21	2.56	0.40
57:CC:91:VAL:HB	57:CC:104:VAL:CG1	2.51	0.40
10:K:71:ARG:HA	10:K:71:ARG:HD3	1.81	0.40
26:1:1592:C:H2'	26:1:1593:A:C8	2.56	0.40
26:1:2139:U:H2'	26:1:2140:G:C8	2.56	0.40
27:2:662:U:H2'	27:2:663:A:C8	2.56	0.40
29:5:31:G:H2'	29:5:32:4OC:H6	2.03	0.40
32:c:13:SER:HB2	32:c:49:TYR:CZ	2.56	0.40
36:g:43:LEU:HD23	36:g:43:LEU:HA	1.88	0.40
37:h:85:GLU:OE2	37:h:88:ARG:NH2	2.44	0.40
47:r:78:LYS:HE3	47:r:78:LYS:HB3	1.95	0.40
3:D:3:LEU:O	3:D:12:LEU:N	2.47	0.40
4:E:38:MET:HE2	4:E:38:MET:HB3	1.94	0.40
15:P:13:MET:HE2	15:P:55:LEU:N	2.35	0.40
17:R:2:TYR:CZ	17:R:42:ALA:HB3	2.56	0.40
26:1:414:C:H2'	26:1:415:A:C8	2.57	0.40
26:1:813:U:H2'	26:1:814:C:C6	2.55	0.40
26:1:1720:U:H2'	26:1:1721:G:O4'	2.22	0.40
26:1:2591:C:H2'	26:1:2592:G:H8	1.85	0.40
27:2:713:G:H2'	27:2:714:G:C8	2.56	0.40
27:2:911:U:H2'	27:2:912:C:C6	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:g:117:LEU:HA	36:g:117:LEU:HD23	1.90	0.40
6:G:50:ARG:O	6:G:54:LEU:HG	2.21	0.40
26:1:570:G:H2'	26:1:2030:6MZ:N7	2.36	0.40
26:1:708:G:N2	26:1:724:U:H1'	2.36	0.40
26:1:1042:G:O2'	26:1:1043:C:H6	2.05	0.40
27:2:94:G:H1'	27:2:95:C:C5	2.56	0.40
27:2:328:C:H2'	27:2:328:C:O2	2.22	0.40
30:a:8:LYS:HA	30:a:8:LYS:HD2	1.88	0.40
30:a:56:ARG:HH12	30:a:59:ARG:NH1	2.19	0.40
3:D:69:ARG:HD3	26:1:674:G:H1'	2.04	0.40
3:D:172:ALA:O	3:D:199:MET:HE1	2.21	0.40
8:I:39:LYS:HE2	8:I:39:LYS:HB3	1.87	0.40
9:J:34:ARG:HG3	9:J:39:LYS:HB2	2.03	0.40
26:1:172:A:H2'	26:1:173:A:C8	2.57	0.40
26:1:2025:C:H2'	26:1:2026:U:C6	2.57	0.40
26:1:2125:G:H22	26:1:2171:A:P	2.45	0.40
26:1:2243:U:H2'	26:1:2244:U:C6	2.57	0.40
27:2:1390:U:H2'	27:2:1391:U:C6	2.57	0.40
28:3:48:U:H2'	28:3:49:C:C6	2.57	0.40
41:l:11:LYS:HE3	41:l:11:LYS:HB2	1.86	0.40
41:l:99:LEU:HD23	41:l:99:LEU:HA	1.87	0.40
57:AA:58:GLY:HA2	57:AA:126:TYR:CE1	2.57	0.40
57:BB:106:LYS:HE2	57:BB:106:LYS:HB3	1.91	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	B	269/273 (98%)	262 (97%)	7 (3%)	0	100	100
2	C	207/209 (99%)	202 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
4	E	175/179 (98%)	173 (99%)	2 (1%)	0	100	100
5	F	173/177 (98%)	169 (98%)	4 (2%)	0	100	100
6	G	147/149 (99%)	140 (95%)	7 (5%)	0	100	100
7	H	128/165 (78%)	108 (84%)	20 (16%)	0	100	100
8	I	133/142 (94%)	121 (91%)	12 (9%)	0	100	100
9	J	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
10	K	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
11	L	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
12	M	134/136 (98%)	134 (100%)	0	0	100	100
13	N	117/127 (92%)	114 (97%)	3 (3%)	0	100	100
14	O	114/117 (97%)	114 (100%)	0	0	100	100
15	P	112/115 (97%)	112 (100%)	0	0	100	100
16	Q	115/118 (98%)	115 (100%)	0	0	100	100
17	R	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
18	S	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
19	T	92/100 (92%)	91 (99%)	1 (1%)	0	100	100
20	U	101/104 (97%)	97 (96%)	4 (4%)	0	100	100
21	V	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
22	W	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
23	X	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
24	Y	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
25	Z	56/59 (95%)	56 (100%)	0	0	100	100
30	a	64/70 (91%)	62 (97%)	2 (3%)	0	100	100
31	b	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
32	c	50/55 (91%)	50 (100%)	0	0	100	100
33	d	44/46 (96%)	44 (100%)	0	0	100	100
34	e	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
35	f	36/38 (95%)	36 (100%)	0	0	100	100
36	g	223/241 (92%)	218 (98%)	5 (2%)	0	100	100
37	h	206/233 (88%)	201 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	i	203/206 (98%)	203 (100%)	0	0	100	100
39	j	154/167 (92%)	151 (98%)	3 (2%)	0	100	100
40	k	102/135 (76%)	102 (100%)	0	0	100	100
41	l	149/179 (83%)	146 (98%)	3 (2%)	0	100	100
42	m	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
43	n	125/130 (96%)	118 (94%)	7 (6%)	0	100	100
44	o	97/103 (94%)	88 (91%)	9 (9%)	0	100	100
45	p	115/129 (89%)	111 (96%)	4 (4%)	0	100	100
46	q	120/124 (97%)	117 (98%)	3 (2%)	0	100	100
47	r	114/118 (97%)	110 (96%)	4 (4%)	0	100	100
48	s	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
49	t	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
50	u	80/82 (98%)	79 (99%)	1 (1%)	0	100	100
51	v	78/84 (93%)	77 (99%)	1 (1%)	0	100	100
52	w	64/75 (85%)	62 (97%)	2 (3%)	0	100	100
53	x	81/92 (88%)	81 (100%)	0	0	100	100
54	y	84/87 (97%)	84 (100%)	0	0	100	100
55	z	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
57	AA	125/152 (82%)	119 (95%)	6 (5%)	0	100	100
57	BB	130/152 (86%)	125 (96%)	5 (4%)	0	100	100
57	CC	123/152 (81%)	119 (97%)	3 (2%)	1 (1%)	16	27
All	All	6247/6676 (94%)	6085 (97%)	161 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
57	CC	71	PRO

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	216/218 (99%)	210 (97%)	6 (3%)	38	60
2	C	164/164 (100%)	160 (98%)	4 (2%)	43	65
3	D	165/165 (100%)	159 (96%)	6 (4%)	31	51
4	E	148/150 (99%)	141 (95%)	7 (5%)	23	40
5	F	136/138 (99%)	130 (96%)	6 (4%)	25	43
6	G	114/114 (100%)	103 (90%)	11 (10%)	8	12
7	H	99/123 (80%)	93 (94%)	6 (6%)	17	30
8	I	104/110 (94%)	96 (92%)	8 (8%)	12	20
9	J	116/116 (100%)	113 (97%)	3 (3%)	40	63
10	K	104/104 (100%)	100 (96%)	4 (4%)	29	49
11	L	103/103 (100%)	100 (97%)	3 (3%)	37	58
12	M	109/109 (100%)	105 (96%)	4 (4%)	30	50
13	N	99/103 (96%)	97 (98%)	2 (2%)	48	69
14	O	86/87 (99%)	86 (100%)	0	100	100
15	P	99/100 (99%)	96 (97%)	3 (3%)	36	57
16	Q	89/90 (99%)	86 (97%)	3 (3%)	32	53
17	R	84/84 (100%)	81 (96%)	3 (4%)	31	51
18	S	93/93 (100%)	90 (97%)	3 (3%)	34	55
19	T	81/84 (96%)	80 (99%)	1 (1%)	63	79
20	U	84/85 (99%)	82 (98%)	2 (2%)	43	65
21	V	78/78 (100%)	77 (99%)	1 (1%)	61	77
22	W	58/63 (92%)	57 (98%)	1 (2%)	53	73
23	X	67/68 (98%)	66 (98%)	1 (2%)	57	75
24	Y	54/55 (98%)	52 (96%)	2 (4%)	30	50
25	Z	48/49 (98%)	46 (96%)	2 (4%)	26	45
30	a	59/62 (95%)	56 (95%)	3 (5%)	21	36
31	b	47/48 (98%)	47 (100%)	0	100	100
32	c	47/49 (96%)	47 (100%)	0	100	100
33	d	38/38 (100%)	38 (100%)	0	100	100
34	e	51/52 (98%)	50 (98%)	1 (2%)	48	69
35	f	34/34 (100%)	34 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	g	187/199 (94%)	185 (99%)	2 (1%)	65	80
37	h	171/190 (90%)	168 (98%)	3 (2%)	51	72
38	i	172/173 (99%)	168 (98%)	4 (2%)	44	66
39	j	119/126 (94%)	115 (97%)	4 (3%)	32	53
40	k	91/116 (78%)	85 (93%)	6 (7%)	15	26
41	l	124/147 (84%)	119 (96%)	5 (4%)	28	47
42	m	104/105 (99%)	102 (98%)	2 (2%)	50	71
43	n	105/107 (98%)	99 (94%)	6 (6%)	18	32
44	o	86/90 (96%)	82 (95%)	4 (5%)	23	40
45	p	90/99 (91%)	89 (99%)	1 (1%)	65	80
46	q	102/103 (99%)	99 (97%)	3 (3%)	37	58
47	r	94/96 (98%)	93 (99%)	1 (1%)	65	80
48	s	83/84 (99%)	83 (100%)	0	100	100
49	t	76/77 (99%)	72 (95%)	4 (5%)	20	35
50	u	65/65 (100%)	63 (97%)	2 (3%)	35	56
51	v	74/78 (95%)	71 (96%)	3 (4%)	27	46
52	w	57/65 (88%)	56 (98%)	1 (2%)	51	72
53	x	72/79 (91%)	70 (97%)	2 (3%)	38	60
54	y	65/66 (98%)	65 (100%)	0	100	100
55	z	60/61 (98%)	59 (98%)	1 (2%)	53	73
57	AA	115/138 (83%)	114 (99%)	1 (1%)	70	82
57	BB	120/138 (87%)	120 (100%)	0	100	100
57	CC	113/138 (82%)	111 (98%)	2 (2%)	51	72
All	All	5219/5476 (95%)	5066 (97%)	153 (3%)	38	58

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	3	VAL
1	B	35	GLU
1	B	139	SER
1	B	156	ARG
1	B	180	GLU
1	B	202	LEU

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Mol	Chain	Res	Type
2	C	59	ARG
2	C	104	VAL
2	C	151	THR
2	C	170	VAL
3	D	4	VAL
3	D	69	ARG
3	D	109	LEU
3	D	150	THR
3	D	152	GLU
3	D	153	LEU
4	E	28	VAL
4	E	44	ILE
4	E	105	THR
4	E	132	VAL
4	E	140	GLU
4	E	149	VAL
4	E	174	ASP
5	F	11	VAL
5	F	43	VAL
5	F	49	THR
5	F	92	VAL
5	F	127	THR
5	F	168	VAL
6	G	3	VAL
6	G	9	VAL
6	G	17	ASP
6	G	66	ASN
6	G	68	ARG
6	G	78	VAL
6	G	110	VAL
6	G	121	VAL
6	G	130	VAL
6	G	143	ILE
6	G	146	VAL
7	H	50	VAL
7	H	53	ARG
7	H	55	VAL
7	H	59	LEU
7	H	67	THR
7	H	118	ILE
8	I	9	LYS
8	I	10	LEU

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Mol	Chain	Res	Type
8	I	11	GLN
8	I	16	MET
8	I	20	SER
8	I	48	ILE
8	I	49	GLU
8	I	117	THR
9	J	11	VAL
9	J	30	THR
9	J	81	ILE
10	K	58	LEU
10	K	67	LYS
10	K	70	ARG
10	K	76	VAL
11	L	60	ARG
11	L	86	GLU
11	L	120	VAL
12	M	75	GLU
12	M	88	ASN
12	M	112	LEU
12	M	126	ILE
13	N	51	LEU
13	N	95	THR
15	P	40	LEU
15	P	71	GLU
15	P	81	VAL
16	Q	51	ARG
16	Q	89	GLU
16	Q	92	ARG
17	R	51	VAL
17	R	58	VAL
17	R	86	GLN
18	S	19	LEU
18	S	97	LEU
18	S	107	VAL
19	T	25	GLU
20	U	39	ILE
20	U	54	GLN
21	V	62	THR
22	W	70	GLU
23	X	11	ARG
24	Y	8	GLU
24	Y	24	GLU

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Mol	Chain	Res	Type
25	Z	32	ILE
25	Z	36	VAL
30	a	32	LEU
30	a	51	VAL
30	a	62	LYS
34	e	33	LEU
36	g	135	LEU
36	g	161	LEU
37	h	33	LEU
37	h	52	VAL
37	h	129	MET
38	i	30	THR
38	i	129	VAL
38	i	143	VAL
38	i	160	GLU
39	j	94	VAL
39	j	114	VAL
39	j	115	LEU
39	j	120	VAL
40	k	1	MET
40	k	76	THR
40	k	84	VAL
40	k	88	MET
40	k	89	VAL
40	k	96	VAL
41	l	6	VAL
41	l	7	ILE
41	l	23	LEU
41	l	50	LEU
41	l	106	GLU
42	m	51	VAL
42	m	90	ASP
43	n	19	VAL
43	n	25	ASN
43	n	43	THR
43	n	53	GLU
43	n	58	VAL
43	n	116	VAL
44	o	17	LEU
44	o	31	ARG
44	o	74	VAL
44	o	76	ILE

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Mol	Chain	Res	Type
45	p	30	THR
46	q	4	VAL
46	q	52	VAL
46	q	74	LEU
47	r	16	VAL
49	t	18	ASP
49	t	22	THR
49	t	39	LEU
49	t	67	LEU
50	u	2	VAL
50	u	3	THR
51	v	39	LYS
51	v	67	LEU
51	v	79	VAL
52	w	74	HIS
53	x	20	GLU
53	x	56	GLN
55	z	6	VAL
57	AA	96	ILE
57	CC	79	VAL
57	CC	101	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	25	HIS
1	B	134	ASN
2	C	94	GLN
3	D	9	GLN
3	D	46	GLN
3	D	94	GLN
5	F	48	ASN
5	F	104	ASN
6	G	119	ASN
9	J	86	GLN
12	M	60	GLN
15	P	3	ASN
20	U	69	ASN
22	W	57	HIS
23	X	6	GLN
24	Y	38	GLN
24	Y	39	GLN

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Mol	Chain	Res	Type
30	a	33	ASN
33	d	26	ASN
33	d	29	GLN
36	g	39	HIS
36	g	58	ASN
36	g	227	GLN
38	i	131	ASN
38	i	164	GLN
39	j	122	ASN
40	k	58	HIS
40	k	94	HIS
41	l	148	ASN
43	n	31	ASN
44	o	20	GLN
45	p	38	GLN
45	p	81	ASN
45	p	118	HIS
45	p	119	ASN
48	s	4	GLN
49	t	50	HIS
50	u	29	ASN
50	u	59	HIS
50	u	79	ASN
54	y	61	GLN
54	y	84	ASN
57	AA	51	GLN
57	AA	105	GLN
57	CC	85	HIS
57	CC	105	GLN
57	CC	120	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
26	1	2902/2904 (99%)	414 (14%)	7 (0%)
27	2	1532/1534 (99%)	209 (13%)	4 (0%)
28	3	119/120 (99%)	12 (10%)	0
29	5	74/77 (96%)	14 (18%)	2 (2%)
56	XX	7/117 (5%)	2 (28%)	0
All	All	4634/4752 (97%)	651 (14%)	13 (0%)

All (651) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
26	1	10	A
26	1	15	G
26	1	34	U
26	1	46	G
26	1	60	G
26	1	71	A
26	1	74	A
26	1	75	G
26	1	85	G
26	1	101	A
26	1	102	U
26	1	118	A
26	1	119	A
26	1	120	U
26	1	137	U
26	1	139	U
26	1	140	C
26	1	163	C
26	1	181	A
26	1	196	A
26	1	199	A
26	1	215	G
26	1	216	A
26	1	221	A
26	1	222	A
26	1	233	A
26	1	248	G
26	1	265	A
26	1	266	G
26	1	272	A
26	1	275	C
26	1	278	A
26	1	285	G
26	1	291	G
26	1	311	A
26	1	329	G
26	1	330	A
26	1	353	C
26	1	361	G
26	1	367	G
26	1	371	A
26	1	372	G
26	1	380	G

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Mol	Chain	Res	Type
26	1	386	G
26	1	396	G
26	1	405	U
26	1	411	G
26	1	412	A
26	1	424	G
26	1	447	A
26	1	457	A
26	1	471	A
26	1	481	G
26	1	491	G
26	1	505	A
26	1	508	A
26	1	509	C
26	1	530	G
26	1	532	A
26	1	544	C
26	1	546	U
26	1	547	A
26	1	548	G
26	1	549	G
26	1	551	G
26	1	563	A
26	1	573	U
26	1	575	A
26	1	588	U
26	1	603	A
26	1	613	A
26	1	614	A
26	1	615	U
26	1	622	G
26	1	627	A
26	1	637	A
26	1	645	C
26	1	647	G
26	1	653	U
26	1	654	A
26	1	655	A
26	1	686	U
26	1	717	C
26	1	726	G
26	1	730	A

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Mol	Chain	Res	Type
26	1	738	G
26	1	747	5MU
26	1	775	G
26	1	776	G
26	1	782	A
26	1	784	G
26	1	785	G
26	1	789	A
26	1	791	C
26	1	805	G
26	1	812	C
26	1	819	A
26	1	827	U
26	1	828	U
26	1	830	G
26	1	845	A
26	1	846	U
26	1	847	U
26	1	858	G
26	1	859	G
26	1	865	C
26	1	878	A
26	1	880	G
26	1	882	G
26	1	884	U
26	1	885	C
26	1	887	A
26	1	891	G
26	1	895	U
26	1	896	A
26	1	910	A
26	1	914	G
26	1	941	A
26	1	946	C
26	1	961	C
26	1	974	G
26	1	983	A
26	1	995	C
26	1	996	A
26	1	999	U
26	1	1012	U
26	1	1013	C

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Mol	Chain	Res	Type
26	1	1022	G
26	1	1033	U
26	1	1040	A
26	1	1043	C
26	1	1046	A
26	1	1047	G
26	1	1057	A
26	1	1060	U
26	1	1061	U
26	1	1062	G
26	1	1066	U
26	1	1068	G
26	1	1070	A
26	1	1071	G
26	1	1073	A
26	1	1083	U
26	1	1084	A
26	1	1085	A
26	1	1087	G
26	1	1088	A
26	1	1090	A
26	1	1095	A
26	1	1097	U
26	1	1101	U
26	1	1106	G
26	1	1111	A
26	1	1112	G
26	1	1122	G
26	1	1132	U
26	1	1133	A
26	1	1134	A
26	1	1135	C
26	1	1142	A
26	1	1169	A
26	1	1170	C
26	1	1172	C
26	1	1173	U
26	1	1175	A
26	1	1176	U
26	1	1177	G
26	1	1178	C
26	1	1179	G

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Mol	Chain	Res	Type
26	1	1182	G
26	1	1206	G
26	1	1212	G
26	1	1236	G
26	1	1238	G
26	1	1253	A
26	1	1256	G
26	1	1266	G
26	1	1271	G
26	1	1272	A
26	1	1300	G
26	1	1301	A
26	1	1314	C
26	1	1329	U
26	1	1341	G
26	1	1352	U
26	1	1365	A
26	1	1368	G
26	1	1379	U
26	1	1380	G
26	1	1383	A
26	1	1386	C
26	1	1407	G
26	1	1409	U
26	1	1411	U
26	1	1416	G
26	1	1417	C
26	1	1428	C
26	1	1437	C
26	1	1452	G
26	1	1453	A
26	1	1460	U
26	1	1482	G
26	1	1490	A
26	1	1493	C
26	1	1503	A
26	1	1508	A
26	1	1510	G
26	1	1515	A
26	1	1524	G
26	1	1532	A
26	1	1535	A

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Mol	Chain	Res	Type
26	1	1536	C
26	1	1537	G
26	1	1566	A
26	1	1569	A
26	1	1578	U
26	1	1580	A
26	1	1583	A
26	1	1584	U
26	1	1586	A
26	1	1589	U
26	1	1590	A
26	1	1607	C
26	1	1608	A
26	1	1610	A
26	1	1618	6MZ
26	1	1626	A
26	1	1634	A
26	1	1647	U
26	1	1648	U
26	1	1649	G
26	1	1674	G
26	1	1715	G
26	1	1729	U
26	1	1730	C
26	1	1738	G
26	1	1764	C
26	1	1773	A
26	1	1782	U
26	1	1800	C
26	1	1801	A
26	1	1802	A
26	1	1808	A
26	1	1811	G
26	1	1816	C
26	1	1829	A
26	1	1833	C
26	1	1847	A
26	1	1848	A
26	1	1870	C
26	1	1871	A
26	1	1872	A
26	1	1906	G

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Mol	Chain	Res	Type
26	1	1914	C
26	1	1915	3TD
26	1	1923	U
26	1	1924	C
26	1	1929	G
26	1	1930	G
26	1	1936	A
26	1	1938	A
26	1	1955	U
26	1	1967	C
26	1	1970	A
26	1	1971	U
26	1	1972	G
26	1	1991	U
26	1	1993	U
26	1	1997	C
26	1	2022	U
26	1	2023	C
26	1	2030	6MZ
26	1	2031	A
26	1	2033	A
26	1	2043	C
26	1	2055	C
26	1	2056	G
26	1	2060	A
26	1	2061	G
26	1	2062	A
26	1	2069	G7M
26	1	2093	G
26	1	2099	U
26	1	2100	G
26	1	2110	G
26	1	2111	U
26	1	2113	U
26	1	2115	G
26	1	2116	G
26	1	2117	A
26	1	2118	U
26	1	2120	G
26	1	2125	G
26	1	2126	A
26	1	2127	G

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Mol	Chain	Res	Type
26	1	2128	G
26	1	2131	U
26	1	2132	U
26	1	2133	G
26	1	2134	A
26	1	2139	U
26	1	2146	C
26	1	2147	A
26	1	2148	G
26	1	2157	G
26	1	2158	A
26	1	2162	G
26	1	2164	C
26	1	2171	A
26	1	2172	U
26	1	2182	U
26	1	2183	A
26	1	2189	U
26	1	2194	U
26	1	2198	A
26	1	2204	G
26	1	2211	A
26	1	2212	A
26	1	2225	A
26	1	2226	C
26	1	2238	G
26	1	2239	G
26	1	2250	G
26	1	2268	A
26	1	2278	A
26	1	2283	C
26	1	2286	G
26	1	2287	A
26	1	2288	A
26	1	2305	U
26	1	2309	A
26	1	2322	A
26	1	2325	G
26	1	2327	A
26	1	2333	A
26	1	2336	A
26	1	2345	G

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Mol	Chain	Res	Type
26	1	2347	C
26	1	2350	C
26	1	2361	G
26	1	2383	G
26	1	2385	C
26	1	2389	G
26	1	2402	U
26	1	2403	C
26	1	2406	A
26	1	2423	U
26	1	2424	C
26	1	2425	A
26	1	2426	A
26	1	2429	G
26	1	2430	A
26	1	2431	U
26	1	2434	A
26	1	2441	U
26	1	2445	2MG
26	1	2448	A
26	1	2470	G
26	1	2476	A
26	1	2478	A
26	1	2491	U
26	1	2498	OMC
26	1	2502	G
26	1	2505	G
26	1	2506	U
26	1	2518	A
26	1	2520	C
26	1	2525	G
26	1	2529	G
26	1	2549	G
26	1	2554	U
26	1	2566	A
26	1	2567	G
26	1	2573	C
26	1	2601	C
26	1	2602	A
26	1	2603	G
26	1	2609	U
26	1	2613	U

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Mol	Chain	Res	Type
26	1	2615	U
26	1	2629	U
26	1	2630	G
26	1	2635	A
26	1	2638	G
26	1	2646	C
26	1	2663	G
26	1	2689	U
26	1	2690	U
26	1	2707	U
26	1	2714	G
26	1	2716	C
26	1	2726	A
26	1	2733	A
26	1	2744	G
26	1	2748	A
26	1	2757	A
26	1	2777	G
26	1	2778	A
26	1	2791	G
26	1	2793	C
26	1	2794	C
26	1	2796	U
26	1	2818	U
26	1	2820	A
26	1	2821	A
26	1	2835	A
26	1	2843	G
26	1	2861	U
26	1	2867	G
26	1	2873	A
26	1	2880	C
26	1	2883	A
26	1	2884	U
26	1	2885	G
27	2	9	G
27	2	32	A
27	2	39	G
27	2	47	C
27	2	48	C
27	2	50	A
27	2	51	A

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Mol	Chain	Res	Type
27	2	54	C
27	2	68	G
27	2	70	U
27	2	72	A
27	2	73	C
27	2	74	A
27	2	77	A
27	2	78	A
27	2	83	C
27	2	84	U
27	2	85	U
27	2	87	C
27	2	94	G
27	2	95	C
27	2	100	G
27	2	120	A
27	2	121	U
27	2	128	G
27	2	130	A
27	2	131	A
27	2	141	G
27	2	181	A
27	2	182	A
27	2	204	G
27	2	209	U
27	2	211	G
27	2	212	G
27	2	245	U
27	2	247	G
27	2	251	G
27	2	266	G
27	2	267	C
27	2	279	A
27	2	280	C
27	2	289	G
27	2	306	A
27	2	321	A
27	2	328	C
27	2	332	G
27	2	352	C
27	2	354	G
27	2	367	U

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Mol	Chain	Res	Type
27	2	372	C
27	2	373	A
27	2	384	G
27	2	398	U
27	2	406	G
27	2	411	A
27	2	412	A
27	2	413	G
27	2	414	A
27	2	421	U
27	2	422	C
27	2	424	G
27	2	429	U
27	2	436	C
27	2	457	G
27	2	458	U
27	2	463	U
27	2	467	U
27	2	468	A
27	2	481	G
27	2	482	A
27	2	484	G
27	2	486	U
27	2	495	A
27	2	496	A
27	2	497	G
27	2	509	A
27	2	511	C
27	2	517	G
27	2	518	C
27	2	519	C
27	2	532	A
27	2	533	A
27	2	536	C
27	2	547	A
27	2	559	A
27	2	572	A
27	2	573	A
27	2	576	C
27	2	579	A
27	2	633	G
27	2	639	G

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Mol	Chain	Res	Type
27	2	653	U
27	2	665	A
27	2	695	A
27	2	700	G
27	2	703	G
27	2	721	G
27	2	723	U
27	2	724	G
27	2	731	G
27	2	734	G
27	2	747	A
27	2	748	G
27	2	755	G
27	2	777	A
27	2	793	U
27	2	794	A
27	2	815	A
27	2	817	C
27	2	821	G
27	2	828	U
27	2	829	G
27	2	841	C
27	2	844	G
27	2	845	A
27	2	846	G
27	2	851	G
27	2	902	G
27	2	914	A
27	2	926	G
27	2	934	C
27	2	935	A
27	2	960	U
27	2	966	2MG
27	2	969	A
27	2	971	G
27	2	975	A
27	2	976	G
27	2	977	A
27	2	992	U
27	2	993	G
27	2	996	A
27	2	1004	A

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Mol	Chain	Res	Type
27	2	1005	A
27	2	1008	U
27	2	1009	U
27	2	1019	A
27	2	1020	G
27	2	1026	G
27	2	1028	C
27	2	1030	U
27	2	1033	G
27	2	1044	A
27	2	1053	G
27	2	1065	U
27	2	1085	U
27	2	1089	G
27	2	1094	G
27	2	1095	U
27	2	1101	A
27	2	1124	G
27	2	1132	C
27	2	1136	C
27	2	1137	C
27	2	1138	G
27	2	1139	G
27	2	1140	C
27	2	1141	C
27	2	1145	A
27	2	1146	A
27	2	1154	G
27	2	1159	U
27	2	1174	G
27	2	1175	G
27	2	1176	A
27	2	1184	G
27	2	1196	A
27	2	1197	A
27	2	1213	A
27	2	1227	A
27	2	1228	C
27	2	1238	A
27	2	1239	A
27	2	1258	G
27	2	1275	A

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Mol	Chain	Res	Type
27	2	1279	G
27	2	1280	A
27	2	1285	A
27	2	1286	U
27	2	1287	A
27	2	1299	A
27	2	1302	C
27	2	1305	G
27	2	1317	C
27	2	1319	A
27	2	1320	C
27	2	1338	G
27	2	1340	A
27	2	1346	A
27	2	1353	G
27	2	1363	A
27	2	1370	G
27	2	1379	G
27	2	1397	C
27	2	1398	A
27	2	1419	G
27	2	1432	G
27	2	1441	A
27	2	1446	A
27	2	1453	G
27	2	1475	G
27	2	1492	A
27	2	1493	A
27	2	1497	G
27	2	1506	U
27	2	1517	G
27	2	1529	G
27	2	1530	G
27	2	1534	A
28	3	2	G
28	3	13	G
28	3	24	G
28	3	25	U
28	3	35	C
28	3	51	G
28	3	56	G
28	3	84	G

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Mol	Chain	Res	Type
28	3	89	U
28	3	90	C
28	3	99	A
28	3	109	A
29	5	2	C
29	5	8	4SU
29	5	13	A
29	5	16	C
29	5	18	G
29	5	19	G
29	5	20	H2U
29	5	21	A
29	5	22	G
29	5	47	U
29	5	48	C
29	5	54	5MU
29	5	58	A
29	5	74	C
56	XX	5	G
56	XX	8	G

All (13) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	1	404	A
26	1	784	G
26	1	894	U
26	1	1379	U
26	1	2146	C
26	1	2602	A
26	1	2756	U
27	2	428	G
27	2	516	PSU
27	2	1109	C
27	2	1145	A
29	5	17	U
29	5	47	U

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

40 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$
29	8AN	5	76	59,29,58	22,24,25	3.60	9 (40%)	26,35,38	2.54	8 (30%)
26	2MA	1	2503	26,58	22,25,26	3.60	8 (36%)	33,37,40	2.14	10 (30%)
27	7MG	2	527	27	22,26,27	3.26	10 (45%)	29,39,42	1.95	8 (27%)
26	5MU	1	747	26	19,22,23	4.78	7 (36%)	28,32,35	3.41	8 (28%)
29	4SU	5	8	29	18,21,22	3.64	8 (44%)	26,30,33	2.22	5 (19%)
27	UR3	2	1498	27	19,22,23	2.43	6 (31%)	26,32,35	1.43	2 (7%)
26	5MU	1	1939	26,58	19,22,23	4.68	7 (36%)	28,32,35	3.87	12 (42%)
26	OMG	1	2251	26,29	23,26,27	2.33	8 (34%)	33,38,41	2.42	11 (33%)
27	MA6	2	1518	27	23,26,27	1.68	5 (21%)	34,38,41	3.21	11 (32%)
26	PSU	1	1917	26	18,21,22	1.02	2 (11%)	22,30,33	1.66	4 (18%)
26	PSU	1	2605	26	18,21,22	1.15	2 (11%)	22,30,33	1.64	4 (18%)
27	4OC	2	1402	27	20,23,24	2.84	8 (40%)	26,32,35	0.95	1 (3%)
29	PSU	5	55	29	18,21,22	1.04	1 (5%)	22,30,33	1.78	5 (22%)
26	G7M	1	2069	26	23,26,27	2.11	6 (26%)	35,39,42	2.59	11 (31%)
26	3TD	1	1915	26	18,22,23	4.49	7 (38%)	22,32,35	1.71	3 (13%)
27	5MC	2	1407	27	18,22,23	3.19	7 (38%)	26,32,35	1.12	1 (3%)
26	PSU	1	746	26	18,21,22	1.09	1 (5%)	22,30,33	1.70	4 (18%)
26	1MG	1	745	26	22,26,27	2.53	8 (36%)	33,39,42	1.84	8 (24%)
26	PSU	1	955	26	18,21,22	1.15	1 (5%)	22,30,33	2.02	4 (18%)
29	H2U	5	20	29,58	18,21,22	3.54	3 (16%)	21,30,33	2.02	5 (23%)
46	0TD	q	89	46	7,9,10	1.47	0	6,11,13	2.30	2 (33%)
27	2MG	2	1207	27	23,26,27	2.67	8 (34%)	32,38,41	2.24	13 (40%)
26	OMU	1	2552	26	19,22,23	2.65	7 (36%)	26,31,34	2.10	7 (26%)
26	PSU	1	2504	26	18,21,22	1.02	1 (5%)	22,30,33	1.87	4 (18%)
26	OMC	1	2498	26,58	19,22,23	2.69	8 (42%)	26,31,34	0.97	1 (3%)
26	6MZ	1	1618	26	22,25,26	2.34	7 (31%)	30,36,39	2.45	9 (30%)
26	2MG	1	1835	26	23,26,27	2.54	7 (30%)	32,38,41	2.15	9 (28%)
26	PSU	1	1911	26	18,21,22	1.06	1 (5%)	22,30,33	1.70	4 (18%)
27	2MG	2	1516	27	23,26,27	2.64	8 (34%)	32,38,41	2.26	9 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	4OC	5	32	29	20,23,24	2.83	8 (40%)	26,32,35	0.97	2 (7%)
27	PSU	2	516	27,58	18,21,22	1.08	1 (5%)	22,30,33	1.81	3 (13%)
27	5MC	2	967	27	18,22,23	3.33	7 (38%)	26,32,35	1.06	2 (7%)
29	5MU	5	54	29	19,22,23	4.75	7 (36%)	28,32,35	3.65	9 (32%)
27	MA6	2	1519	27	23,26,27	1.64	4 (17%)	34,38,41	3.27	11 (32%)
26	5MC	1	1962	26	18,22,23	3.23	7 (38%)	26,32,35	1.05	2 (7%)
26	2MG	1	2445	26	23,26,27	2.66	8 (34%)	32,38,41	2.24	8 (25%)
26	PSU	1	2580	26,58	18,21,22	1.31	3 (16%)	22,30,33	1.89	4 (18%)
26	6MZ	1	2030	26	22,25,26	2.31	7 (31%)	30,36,39	2.62	11 (36%)
26	PSU	1	2457	26	18,21,22	1.15	1 (5%)	22,30,33	2.13	5 (22%)
27	2MG	2	966	27	23,26,27	2.69	7 (30%)	32,38,41	2.21	8 (25%)

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
29	8AN	5	76	59,29,58	-	3/7/25/26	0/3/3/3
26	2MA	1	2503	26,58	-	2/7/25/26	0/3/3/3
27	7MG	2	527	27	-	2/7/37/38	0/3/3/3
26	5MU	1	747	26	-	0/7/25/26	0/2/2/2
29	4SU	5	8	29	-	4/7/25/26	0/2/2/2
27	UR3	2	1498	27	-	0/7/25/26	0/2/2/2
26	5MU	1	1939	26,58	-	0/7/25/26	0/2/2/2
26	OMG	1	2251	26,29	-	1/9/27/28	0/3/3/3
27	MA6	2	1518	27	-	0/11/29/30	0/3/3/3
26	PSU	1	1917	26	-	0/7/25/26	0/2/2/2
26	PSU	1	2605	26	-	0/7/25/26	0/2/2/2
27	4OC	2	1402	27	-	2/9/29/30	0/2/2/2
29	PSU	5	55	29	-	0/7/25/26	0/2/2/2
26	G7M	1	2069	26	-	1/7/25/26	0/3/3/3
26	3TD	1	1915	26	-	5/7/25/26	0/2/2/2
27	5MC	2	1407	27	-	0/7/25/26	0/2/2/2
26	PSU	1	746	26	-	2/7/25/26	0/2/2/2
26	1MG	1	745	26	-	0/7/25/26	0/3/3/3
26	PSU	1	955	26	-	0/7/25/26	0/2/2/2
29	H2U	5	20	29,58	-	5/7/38/39	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	0TD	q	89	46	-	1/7/12/14	-
27	2MG	2	1207	27	-	0/9/27/28	0/3/3/3
26	OMU	1	2552	26	-	1/9/27/28	0/2/2/2
26	PSU	1	2504	26	-	0/7/25/26	0/2/2/2
26	OMC	1	2498	26,58	-	1/9/27/28	0/2/2/2
26	6MZ	1	1618	26	-	2/9/27/28	0/3/3/3
26	2MG	1	1835	26	-	0/9/27/28	0/3/3/3
26	PSU	1	1911	26	-	0/7/25/26	0/2/2/2
27	2MG	2	1516	27	-	0/9/27/28	0/3/3/3
29	4OC	5	32	29	-	0/9/29/30	0/2/2/2
27	PSU	2	516	27,58	-	2/7/25/26	0/2/2/2
27	5MC	2	967	27	-	0/7/25/26	0/2/2/2
29	5MU	5	54	29	-	2/7/25/26	0/2/2/2
27	MA6	2	1519	27	-	0/11/29/30	0/3/3/3
26	5MC	1	1962	26	-	0/7/25/26	0/2/2/2
26	2MG	1	2445	26	-	2/9/27/28	0/3/3/3
26	PSU	1	2580	26,58	-	0/7/25/26	0/2/2/2
26	6MZ	1	2030	26	-	2/9/27/28	0/3/3/3
26	PSU	1	2457	26	-	0/7/25/26	0/2/2/2
27	2MG	2	966	27	-	2/9/27/28	0/3/3/3

All (221) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1	1915	3TD	C6-C5	14.20	1.51	1.35
29	5	20	H2U	C2-N1	12.18	1.53	1.35
29	5	54	5MU	C2-N1	10.92	1.56	1.38
26	1	2503	2MA	C4-N3	10.91	1.48	1.34
26	1	747	5MU	C2-N1	10.79	1.55	1.38
26	1	747	5MU	C6-N1	10.50	1.56	1.38
29	5	54	5MU	C6-N1	10.25	1.55	1.38
26	1	1939	5MU	C2-N1	10.15	1.54	1.38
29	5	54	5MU	C4-C5	9.75	1.61	1.44
26	1	1939	5MU	C4-C5	9.49	1.60	1.44
26	1	1939	5MU	C4-N3	-9.13	1.21	1.38
26	1	1939	5MU	C6-N1	9.05	1.53	1.38
26	1	747	5MU	C4-C5	9.01	1.59	1.44
26	1	1962	5MC	C6-C5	8.70	1.48	1.34
29	5	76	8AN	O4'-C1'	8.67	1.62	1.42
26	1	1915	3TD	C2-N1	8.60	1.48	1.37
27	2	967	5MC	C6-C5	8.51	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	2	1407	5MC	C6-C5	8.42	1.48	1.34
26	1	747	5MU	C4-N3	-8.23	1.23	1.38
26	1	1618	6MZ	C6-N6	8.12	1.43	1.34
29	5	76	8AN	O4'-C4'	-7.98	1.27	1.45
29	5	8	4SU	C4-N3	7.95	1.46	1.37
29	5	54	5MU	C4-N3	-7.94	1.24	1.38
27	2	527	7MG	C8-N9	7.83	1.50	1.46
27	2	527	7MG	C5-N7	7.44	1.44	1.35
26	1	2030	6MZ	C6-N6	7.30	1.42	1.34
29	5	76	8AN	C2'-C1'	-7.23	1.30	1.53
27	2	966	2MG	C2-N3	7.03	1.45	1.31
26	1	2503	2MA	C2-N3	6.77	1.46	1.34
29	5	8	4SU	C2-N3	6.74	1.50	1.38
27	2	1207	2MG	C2-N3	6.70	1.44	1.31
27	2	1516	2MG	C2-N3	6.62	1.44	1.31
26	1	2445	2MG	C2-N3	6.61	1.44	1.31
29	5	20	H2U	C2-N3	6.50	1.49	1.38
26	1	1835	2MG	C2-N3	6.46	1.44	1.31
29	5	8	4SU	C2-N1	6.09	1.48	1.38
27	2	1402	4OC	C4-N3	6.08	1.43	1.32
29	5	32	4OC	C4-N3	6.06	1.43	1.32
26	1	2552	OMU	C2-N3	6.05	1.48	1.38
27	2	966	2MG	C4-N3	6.03	1.48	1.34
26	1	2552	OMU	C2-N1	5.93	1.48	1.38
27	2	1402	4OC	C6-C5	5.91	1.48	1.35
26	1	747	5MU	C6-C5	5.89	1.44	1.34
27	2	1498	UR3	C2-N1	5.84	1.46	1.38
26	1	2445	2MG	C4-N3	5.84	1.48	1.34
27	2	1207	2MG	C4-N3	5.82	1.48	1.34
26	1	1915	3TD	C2-N3	5.81	1.51	1.38
27	2	967	5MC	C4-N3	5.80	1.43	1.34
29	5	32	4OC	C6-C5	5.77	1.48	1.35
26	1	2069	G7M	C4-N3	5.71	1.47	1.34
27	2	967	5MC	C2-N3	5.64	1.47	1.36
26	1	745	1MG	C4-N3	5.60	1.47	1.34
26	1	2503	2MA	C6-N1	5.59	1.43	1.35
29	5	8	4SU	C6-C5	5.57	1.48	1.35
26	1	2251	OMG	C4-N3	5.54	1.47	1.34
29	5	54	5MU	C6-C5	5.54	1.43	1.34
26	1	2503	2MA	C2-N1	5.53	1.43	1.34
26	1	745	1MG	C2-N2	5.51	1.44	1.34
26	1	1835	2MG	C4-N3	5.49	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1	745	1MG	C2-N3	5.48	1.44	1.34
26	1	2498	OMC	C6-C5	5.42	1.47	1.35
26	1	1962	5MC	C4-N3	5.40	1.43	1.34
27	2	1407	5MC	C4-N3	5.36	1.43	1.34
26	1	1939	5MU	C6-C5	5.35	1.43	1.34
29	5	20	H2U	C4-N3	5.34	1.46	1.37
27	2	1516	2MG	C4-N3	5.32	1.46	1.34
29	5	32	4OC	C2-N3	5.28	1.47	1.36
26	1	2552	OMU	C6-C5	5.25	1.47	1.35
27	2	1498	UR3	C6-C5	5.24	1.47	1.35
27	2	966	2MG	C2-N2	5.21	1.45	1.33
26	1	1962	5MC	C2-N3	5.17	1.46	1.36
27	2	1407	5MC	C2-N3	5.15	1.46	1.36
26	1	2069	G7M	C5-N7	-5.12	1.33	1.39
27	2	1402	4OC	C2-N3	5.08	1.46	1.36
26	1	1915	3TD	C6-N1	5.06	1.44	1.36
26	1	2498	OMC	C2-N3	5.05	1.46	1.36
27	2	1207	2MG	C2-N2	5.00	1.44	1.33
29	5	8	4SU	C4-S4	-4.99	1.58	1.68
27	2	527	7MG	C2-N3	4.86	1.44	1.33
27	2	527	7MG	C4-N3	4.81	1.45	1.34
27	2	1518	MA6	C6-N6	4.68	1.50	1.36
26	1	2503	2MA	C5-C6	4.59	1.53	1.41
26	1	2445	2MG	C2-N2	4.57	1.43	1.33
26	1	2498	OMC	C4-N3	4.54	1.43	1.34
26	1	2251	OMG	C2-N3	4.53	1.44	1.33
27	2	1516	2MG	C2-N2	4.47	1.43	1.33
26	1	2498	OMC	C4-N4	4.45	1.44	1.33
26	1	1835	2MG	C2-N2	4.45	1.43	1.33
29	5	32	4OC	C4-N4	4.41	1.45	1.35
29	5	76	8AN	C6-N6	4.41	1.45	1.34
26	1	1939	5MU	O2-C2	-4.31	1.15	1.23
26	1	2251	OMG	C2-N2	4.31	1.44	1.34
27	2	1519	MA6	C6-N6	4.28	1.49	1.36
27	2	1207	2MG	C2-N1	4.28	1.43	1.36
26	1	2030	6MZ	C5-N7	-4.27	1.31	1.39
27	2	1402	4OC	C4-N4	4.23	1.44	1.35
27	2	527	7MG	C2-N2	4.23	1.44	1.34
27	2	967	5MC	C6-N1	4.23	1.45	1.38
27	2	1498	UR3	C2-N3	4.17	1.47	1.39
27	2	1519	MA6	C5-C4	-4.16	1.31	1.39
26	1	1962	5MC	C6-N1	4.13	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1	2498	OMC	C2-N1	4.13	1.48	1.40
27	2	967	5MC	C4-N4	4.06	1.44	1.34
27	2	1516	2MG	C5-N7	-4.05	1.31	1.39
27	2	1407	5MC	C6-N1	4.05	1.45	1.38
26	1	1835	2MG	C5-N7	-4.00	1.31	1.39
29	5	8	4SU	C5-C4	3.99	1.47	1.42
27	2	1518	MA6	C5-C4	-3.94	1.31	1.39
29	5	76	8AN	C5-C4	-3.93	1.31	1.39
26	1	745	1MG	C5-N7	-3.91	1.31	1.39
26	1	2445	2MG	C5-N7	-3.86	1.31	1.39
27	2	966	2MG	C5-N7	-3.84	1.31	1.39
27	2	1516	2MG	C2-N1	3.83	1.42	1.36
27	2	966	2MG	C2-N1	3.80	1.42	1.36
27	2	1407	5MC	C4-N4	3.77	1.43	1.34
26	1	1618	6MZ	C5-N7	-3.76	1.31	1.39
29	5	76	8AN	C8-N9	-3.75	1.30	1.37
27	2	527	7MG	C4-N9	3.74	1.42	1.37
26	1	1962	5MC	C4-N4	3.73	1.43	1.34
27	2	967	5MC	C2-N1	3.73	1.48	1.40
26	1	2251	OMG	O6-C6	-3.72	1.16	1.23
26	1	2445	2MG	O6-C6	-3.71	1.16	1.23
27	2	1407	5MC	C2-N1	3.56	1.47	1.40
27	2	1402	4OC	C5-C4	3.54	1.48	1.40
29	5	32	4OC	C2-N1	3.50	1.47	1.40
27	2	1402	4OC	O2-C2	-3.48	1.17	1.23
26	1	1835	2MG	O6-C6	-3.47	1.17	1.23
26	1	1962	5MC	O2-C2	-3.47	1.17	1.23
29	5	32	4OC	C5-C4	3.44	1.48	1.40
26	1	2030	6MZ	C5-C4	-3.40	1.32	1.39
26	1	747	5MU	O4-C4	-3.40	1.17	1.23
26	1	2251	OMG	C5-N7	-3.38	1.32	1.39
27	2	1516	2MG	O6-C6	-3.37	1.17	1.23
26	1	1618	6MZ	C5-C4	-3.34	1.32	1.39
27	2	1207	2MG	C5-N7	-3.31	1.32	1.39
27	2	1402	4OC	C2-N1	3.28	1.47	1.40
26	1	1835	2MG	C2-N1	3.27	1.42	1.36
27	2	527	7MG	O6-C6	-3.26	1.17	1.23
29	5	76	8AN	C5-N7	-3.25	1.32	1.39
26	1	2503	2MA	C6-N6	-3.25	1.26	1.34
27	2	1407	5MC	O2-C2	-3.23	1.17	1.23
27	2	967	5MC	O2-C2	-3.22	1.17	1.23
29	5	8	4SU	C6-N1	3.19	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	2	1516	2MG	C4-N9	-3.18	1.29	1.38
26	1	2552	OMU	C4-N3	3.15	1.44	1.38
26	1	1939	5MU	O4-C4	-3.14	1.17	1.23
26	1	1962	5MC	C2-N1	3.13	1.46	1.40
26	1	2251	OMG	C4-N9	-3.13	1.29	1.38
26	1	2069	G7M	C2-N2	3.13	1.41	1.34
26	1	2498	OMC	C6-N1	3.09	1.45	1.38
27	2	527	7MG	C2-N1	3.08	1.45	1.37
26	1	1915	3TD	O2-C2	-3.07	1.17	1.23
27	2	527	7MG	C5-C6	3.07	1.51	1.43
26	1	746	PSU	C6-C5	3.06	1.38	1.35
29	5	32	4OC	O2-C2	-3.06	1.18	1.23
26	1	2552	OMU	O4-C4	-3.05	1.18	1.24
26	1	747	5MU	O2-C2	-3.05	1.17	1.23
29	5	55	PSU	C6-C5	3.04	1.38	1.35
26	1	2445	2MG	C4-N9	-3.03	1.30	1.38
26	1	2069	G7M	C4-N9	-3.02	1.30	1.38
26	1	2445	2MG	C2-N1	3.01	1.41	1.36
26	1	2030	6MZ	C4-N9	-3.00	1.31	1.37
26	1	745	1MG	O6-C6	-3.00	1.16	1.23
27	2	1498	UR3	O2-C2	-2.96	1.17	1.22
27	2	1402	4OC	C6-N1	2.94	1.45	1.38
27	2	1498	UR3	O4-C4	-2.92	1.17	1.23
29	5	8	4SU	O2-C2	-2.92	1.17	1.23
27	2	966	2MG	O6-C6	-2.90	1.18	1.23
26	1	2503	2MA	C5-N7	-2.90	1.33	1.39
26	1	1911	PSU	C6-C5	2.89	1.38	1.35
26	1	1618	6MZ	C6-N1	-2.83	1.30	1.35
27	2	1207	2MG	O6-C6	-2.82	1.18	1.23
27	2	516	PSU	C6-C5	2.80	1.38	1.35
26	1	2498	OMC	O2-C2	-2.78	1.18	1.23
29	5	76	8AN	C3'-N3'	-2.74	1.43	1.47
29	5	54	5MU	O4-C4	-2.73	1.18	1.23
26	1	745	1MG	C5-C6	2.70	1.52	1.45
26	1	1917	PSU	C6-C5	2.66	1.38	1.35
26	1	2030	6MZ	C9-N6	-2.66	1.40	1.45
26	1	2580	PSU	O4'-C1'	-2.65	1.40	1.43
29	5	32	4OC	C6-N1	2.62	1.44	1.38
26	1	2504	PSU	C6-C5	2.59	1.38	1.35
26	1	1915	3TD	O4-C4	-2.58	1.17	1.23
26	1	2030	6MZ	C8-N9	-2.55	1.32	1.37
27	2	1498	UR3	C6-N1	2.55	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1	1915	3TD	C4-N3	2.52	1.45	1.40
26	1	2069	G7M	C5-C6	2.51	1.50	1.43
26	1	2457	PSU	C6-C5	2.47	1.38	1.35
29	5	54	5MU	O2-C2	-2.47	1.18	1.23
27	2	1207	2MG	C4-N9	-2.46	1.31	1.38
26	1	2069	G7M	C2-N3	2.45	1.39	1.33
26	1	745	1MG	C4-N9	-2.44	1.31	1.38
26	1	1835	2MG	C4-N9	-2.44	1.31	1.38
26	1	2251	OMG	C2-N1	2.42	1.43	1.37
26	1	2580	PSU	C6-C5	2.41	1.38	1.35
26	1	1618	6MZ	C8-N9	-2.40	1.33	1.37
26	1	2605	PSU	C6-C5	2.39	1.38	1.35
27	2	1207	2MG	C5-C6	2.35	1.53	1.44
26	1	2030	6MZ	C5-C6	-2.32	1.35	1.41
26	1	2445	2MG	C5-C6	2.32	1.53	1.44
27	2	1518	MA6	C8-N9	-2.27	1.33	1.37
27	2	527	7MG	C6-N1	2.27	1.43	1.38
26	1	2552	OMU	O2-C2	-2.27	1.18	1.23
26	1	2580	PSU	C4-C5	-2.27	1.37	1.44
29	5	76	8AN	O2'-C2'	2.26	1.48	1.43
26	1	1618	6MZ	C9-N6	-2.25	1.41	1.45
27	2	1519	MA6	C8-N9	-2.24	1.33	1.37
27	2	1519	MA6	C5-N7	-2.18	1.34	1.39
26	1	2552	OMU	C6-N1	2.16	1.43	1.38
26	1	2498	OMC	C5-C4	2.16	1.47	1.42
26	1	745	1MG	C8-N9	-2.15	1.32	1.37
27	2	1516	2MG	C5-C6	2.14	1.52	1.44
26	1	2251	OMG	C5-C6	2.13	1.52	1.44
27	2	1518	MA6	C5-N7	-2.13	1.35	1.39
26	1	2605	PSU	C4-C5	-2.11	1.38	1.44
26	1	1618	6MZ	C5-C6	-2.10	1.36	1.41
26	1	2503	2MA	C5-C4	-2.04	1.35	1.39
26	1	1917	PSU	C4-C5	-2.04	1.38	1.44
27	2	1518	MA6	C4-N9	-2.04	1.33	1.37
27	2	966	2MG	C5-C6	2.03	1.51	1.44
26	1	955	PSU	O4'-C1'	-2.00	1.41	1.43

All (248) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	2	1519	MA6	N1-C6-N6	-13.05	102.81	117.08
27	2	1518	MA6	N1-C6-N6	-12.29	103.64	117.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	5	54	5MU	C5-C4-N3	12.27	125.79	115.31
26	1	747	5MU	C5-C4-N3	11.28	124.94	115.31
26	1	1939	5MU	C5-C4-N3	11.27	124.93	115.31
26	1	1939	5MU	C5-C6-N1	-10.71	112.32	123.34
29	5	54	5MU	C5-C6-N1	-9.98	113.08	123.34
26	1	747	5MU	C5-C6-N1	-8.71	114.38	123.34
26	1	2251	OMG	C1'-N9-C8	-7.53	105.25	126.70
26	1	2069	G7M	CN7-N7-C5	7.29	135.83	126.77
26	1	2503	2MA	C5-C4-N3	-7.19	119.11	127.19
29	5	8	4SU	C4-N3-C2	-7.07	120.47	127.34
29	5	20	H2U	C4-N3-C2	-7.03	119.96	125.79
26	1	2030	6MZ	N1-C2-N3	-7.00	117.65	128.60
27	2	966	2MG	C2-N3-C4	6.78	120.45	112.04
26	1	1835	2MG	C2-N3-C4	6.75	120.41	112.04
27	2	1207	2MG	C2-N3-C4	6.54	120.15	112.04
26	1	2251	OMG	C1'-N9-C4	6.52	145.87	126.50
27	2	1519	MA6	C5-C6-N6	6.50	136.62	125.30
26	1	2552	OMU	C4-N3-C2	-6.41	118.13	126.58
27	2	1516	2MG	C2-N3-C4	6.36	119.92	112.04
26	1	2445	2MG	C2-N3-C4	6.29	119.84	112.04
27	2	1518	MA6	C5-C6-N6	6.19	136.09	125.30
26	1	747	5MU	O4-C4-C5	-6.18	117.73	124.90
26	1	1618	6MZ	C5-C4-N3	-6.16	118.71	126.75
26	1	1939	5MU	N3-C2-N1	6.11	123.00	114.89
29	5	76	8AN	N1-C2-N3	-6.02	119.19	128.60
26	1	2069	G7M	CN7-N7-C8	-6.02	115.56	124.84
27	2	1518	MA6	N1-C2-N3	-5.90	119.37	128.60
26	1	2457	PSU	N1-C2-N3	5.84	121.74	115.13
27	2	966	2MG	C5-C4-N3	-5.84	118.99	128.46
26	1	2445	2MG	C5-C4-N3	-5.82	119.02	128.46
27	2	1498	UR3	C4-N3-C2	-5.68	119.21	124.56
26	1	1939	5MU	C4-N3-C2	-5.66	120.03	127.35
27	2	1516	2MG	C2-N1-C6	-5.59	118.05	124.48
26	1	1618	6MZ	N1-C2-N3	-5.58	119.87	128.60
26	1	2069	G7M	C1'-N9-C4	5.55	142.97	126.50
26	1	2445	2MG	C2-N1-C6	-5.45	118.20	124.48
26	1	2504	PSU	C4-N3-C2	-5.44	118.51	126.34
26	1	1835	2MG	C5-C4-N3	-5.43	119.66	128.46
26	1	1915	3TD	N1-C2-N3	5.42	120.42	116.14
26	1	2457	PSU	C4-N3-C2	-5.41	118.54	126.34
27	2	1519	MA6	N1-C2-N3	-5.41	120.15	128.60
26	1	955	PSU	C4-N3-C2	-5.40	118.56	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1	745	1MG	C5-C4-N3	-5.35	119.78	128.46
26	1	955	PSU	N1-C2-N3	5.32	121.16	115.13
26	1	2069	G7M	C1'-N9-C8	-5.30	108.84	126.74
29	5	8	4SU	C5-C4-N3	5.29	119.59	114.69
29	5	54	5MU	O4-C4-C5	-5.19	118.89	124.90
26	1	747	5MU	N3-C2-N1	5.08	121.64	114.89
26	1	2030	6MZ	N9-C8-N7	-5.01	107.06	113.91
27	2	527	7MG	C5-C6-N1	5.01	119.81	110.99
27	2	1207	2MG	C5-C4-N3	-5.00	120.35	128.46
27	2	1516	2MG	C5-C4-N3	-5.00	120.35	128.46
26	1	2580	PSU	N1-C2-N3	4.96	120.75	115.13
27	2	1519	MA6	N9-C8-N7	-4.95	107.14	113.91
29	5	76	8AN	C5-C4-N3	-4.95	120.30	126.75
26	1	1939	5MU	C5M-C5-C6	-4.94	116.25	122.85
27	2	1518	MA6	C5-C4-N3	-4.89	120.36	126.75
27	2	1518	MA6	N9-C8-N7	-4.83	107.30	113.91
26	1	2552	OMU	C5-C4-N3	4.83	122.06	114.84
27	2	516	PSU	C4-N3-C2	-4.81	119.40	126.34
27	2	1207	2MG	C2-N1-C6	-4.76	119.00	124.48
27	2	966	2MG	C2-N1-C6	-4.70	119.07	124.48
26	1	2580	PSU	C4-N3-C2	-4.66	119.62	126.34
26	1	2503	2MA	N3-C4-N9	4.66	133.46	126.99
26	1	2605	PSU	C4-N3-C2	-4.60	119.71	126.34
29	5	54	5MU	C4-N3-C2	-4.57	121.43	127.35
27	2	1519	MA6	C5-C4-N3	-4.57	120.79	126.75
26	1	746	PSU	C4-N3-C2	-4.57	119.76	126.34
29	5	55	PSU	N1-C2-N3	4.52	120.25	115.13
26	1	2504	PSU	N1-C2-N3	4.47	120.20	115.13
29	5	55	PSU	C4-N3-C2	-4.46	119.92	126.34
26	1	1618	6MZ	C4-C5-C6	4.41	120.23	116.81
26	1	1835	2MG	C2-N1-C6	-4.41	119.40	124.48
26	1	746	PSU	N1-C2-N3	4.39	120.11	115.13
26	1	1911	PSU	N1-C2-N3	4.39	120.10	115.13
46	q	89	0TD	OD2-CG-CB	4.36	122.56	113.15
26	1	1618	6MZ	N9-C8-N7	-4.35	107.97	113.91
26	1	747	5MU	C4-N3-C2	-4.34	121.74	127.35
26	1	1917	PSU	C4-N3-C2	-4.33	120.11	126.34
29	5	54	5MU	C5M-C5-C4	4.29	123.49	118.77
27	2	516	PSU	N1-C2-N3	4.29	119.98	115.13
26	1	2030	6MZ	C4-N9-C1'	-4.25	116.47	126.59
26	1	1911	PSU	C4-N3-C2	-4.25	120.22	126.34
26	1	2503	2MA	N9-C8-N7	-4.24	108.11	113.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	2	527	7MG	C2-N3-C4	4.22	119.81	112.30
29	5	76	8AN	N6-C6-N1	-4.22	109.12	118.35
29	5	54	5MU	C5M-C5-C6	-4.15	117.31	122.85
26	1	1917	PSU	N1-C2-N3	4.13	119.81	115.13
27	2	1407	5MC	C5-C6-N1	-4.12	119.10	123.34
26	1	2030	6MZ	C5-N7-C8	4.11	109.35	103.51
29	5	76	8AN	N9-C8-N7	-4.06	108.36	113.91
26	1	2030	6MZ	C5-C4-N3	-4.06	121.46	126.75
26	1	745	1MG	C2-N3-C4	3.99	120.95	111.98
26	1	1618	6MZ	N3-C4-N9	3.98	133.63	127.08
26	1	1915	3TD	C4-N3-C2	-3.97	120.30	124.61
26	1	1618	6MZ	C2-N3-C4	3.95	121.08	111.75
26	1	2605	PSU	N1-C2-N3	3.95	119.60	115.13
26	1	2030	6MZ	C2-N3-C4	3.94	121.05	111.75
29	5	54	5MU	N3-C2-N1	3.93	120.11	114.89
26	1	2030	6MZ	C1'-N9-C8	3.89	135.91	127.14
29	5	76	8AN	C5-C6-N6	3.86	131.84	123.43
26	1	1939	5MU	C5M-C5-C4	3.83	122.98	118.77
26	1	2552	OMU	N3-C2-N1	3.75	119.87	114.89
26	1	1939	5MU	O4-C4-C5	-3.75	120.56	124.90
27	2	967	5MC	C5-C6-N1	-3.69	119.54	123.34
27	2	1518	MA6	C2-N3-C4	3.69	120.48	111.75
27	2	966	2MG	N9-C4-N3	3.69	133.36	125.94
26	1	1962	5MC	C5-C6-N1	-3.65	119.58	123.34
26	1	2069	G7M	C5-C6-N1	3.64	119.40	111.79
29	5	8	4SU	N3-C2-N1	3.64	119.72	114.89
26	1	2069	G7M	C2-N3-C4	3.64	118.78	112.30
26	1	745	1MG	N9-C4-N3	3.58	133.13	125.94
27	2	1518	MA6	C2-N1-C6	3.55	120.14	111.75
29	5	76	8AN	C2-N3-C4	3.52	120.08	111.75
26	1	2251	OMG	C2-N3-C4	3.49	118.52	112.30
26	1	2251	OMG	N9-C8-N7	-3.48	106.83	113.39
27	2	527	7MG	C5-C4-N3	-3.48	121.51	128.13
29	5	8	4SU	C1'-N1-C2	3.46	123.83	117.57
26	1	2445	2MG	N9-C4-N3	3.43	132.83	125.94
26	1	1618	6MZ	C5-N7-C8	3.42	108.37	103.51
26	1	1835	2MG	N9-C4-N3	3.41	132.79	125.94
27	2	527	7MG	C5-C4-N9	3.38	110.73	106.35
26	1	747	5MU	C6-N1-C2	-3.38	117.88	121.30
27	2	1519	MA6	C2-N1-C6	3.37	119.72	111.75
27	2	1519	MA6	C2-N3-C4	3.36	119.69	111.75
26	1	1939	5MU	O2-C2-N1	-3.34	118.35	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1	2251	OMG	C5-C4-N3	-3.32	123.07	128.46
27	2	1516	2MG	CM2-N2-C2	-3.32	116.53	123.86
29	5	8	4SU	C5-C4-S4	-3.32	120.19	124.47
26	1	955	PSU	O2-C2-N1	-3.29	119.17	122.79
26	1	1939	5MU	C6-C5-C4	3.27	120.76	118.03
26	1	747	5MU	O2-C2-N1	-3.25	118.46	122.79
27	2	1519	MA6	C4-N9-C8	3.24	109.24	105.73
26	1	2030	6MZ	C4-C5-N7	-3.24	106.68	110.62
27	2	1518	MA6	N3-C4-N9	3.21	132.37	127.08
26	1	745	1MG	N9-C8-N7	-3.17	107.41	113.39
26	1	2503	2MA	N3-C2-N1	-3.14	119.95	125.72
27	2	1519	MA6	C5-N7-C8	3.13	107.96	103.51
27	2	1519	MA6	N3-C4-N9	3.13	132.24	127.08
27	2	1518	MA6	C4-N9-C8	3.13	109.12	105.73
27	2	1518	MA6	C4-C5-C6	3.13	119.38	115.88
27	2	1207	2MG	N9-C8-N7	-3.12	107.51	113.39
26	1	2552	OMU	O4-C4-C5	-3.12	119.67	125.16
27	2	1518	MA6	C5-N7-C8	3.09	107.90	103.51
29	5	20	H2U	N3-C2-N1	3.08	119.91	116.65
26	1	2069	G7M	C5-C4-N3	-3.08	122.25	128.15
26	1	2457	PSU	O2-C2-N1	-3.04	119.44	122.79
26	1	2030	6MZ	C5-C4-N9	3.04	109.32	105.78
26	1	2069	G7M	O6-C6-C5	-3.01	121.26	128.06
27	2	1516	2MG	C5-C6-N1	2.99	120.77	113.19
26	1	2251	OMG	C2'-C1'-N9	-2.96	108.47	114.22
29	5	20	H2U	C5-C4-N3	2.93	119.94	116.65
26	1	1939	5MU	O4-C4-N3	-2.93	114.50	120.12
29	5	76	8AN	C5-N7-C8	2.91	107.65	103.51
26	1	2445	2MG	C5-C6-N1	2.91	120.58	113.19
27	2	1519	MA6	C4-C5-C6	2.86	119.08	115.88
26	1	1939	5MU	C1'-N1-C2	2.85	122.73	117.57
27	2	966	2MG	C5-C6-N1	2.82	120.36	113.19
26	1	1835	2MG	C5-C6-N1	2.82	120.35	113.19
26	1	2069	G7M	C2-N1-C6	-2.81	119.98	125.10
27	2	527	7MG	C4-C5-N7	2.81	109.43	105.53
26	1	2552	OMU	O2-C2-N1	-2.78	119.10	122.79
26	1	745	1MG	C2-N1-C6	-2.77	118.69	120.95
26	1	745	1MG	C5-C6-N1	2.77	120.27	114.91
26	1	2457	PSU	C6-N1-C2	-2.77	119.85	122.68
26	1	2503	2MA	C5-N7-C8	2.76	107.44	103.51
27	2	1207	2MG	C5-C6-N1	2.76	120.20	113.19
26	1	2552	OMU	C2'-C1'-N1	-2.75	108.88	114.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	5	76	8AN	N3-C4-N9	2.75	131.62	127.08
26	1	2498	OMC	O2-C2-N3	-2.74	117.87	122.33
27	2	1516	2MG	N9-C8-N7	-2.73	108.24	113.39
27	2	1516	2MG	O6-C6-C5	-2.65	119.56	126.60
26	1	1962	5MC	CM5-C5-C6	-2.65	119.31	122.85
27	2	527	7MG	O6-C6-C5	-2.64	121.06	127.54
26	1	1917	PSU	O2-C2-N1	-2.64	119.89	122.79
27	2	1207	2MG	N9-C4-N3	2.64	131.23	125.94
27	2	966	2MG	O6-C6-C5	-2.62	119.64	126.60
29	5	55	PSU	O2-C2-N1	-2.62	119.90	122.79
26	1	2504	PSU	O2-C2-N1	-2.62	119.91	122.79
26	1	2503	2MA	N6-C6-N1	2.61	120.72	117.03
26	1	2069	G7M	N2-C2-N1	2.61	122.26	116.71
29	5	20	H2U	C5-C6-N1	2.59	120.16	111.61
27	2	527	7MG	C2-N1-C6	-2.59	120.38	125.10
27	2	1402	4OC	CM4-N4-C4	-2.58	117.41	122.45
27	2	1207	2MG	CM2-N2-C2	-2.58	118.16	123.86
29	5	32	4OC	CM4-N4-C4	-2.55	117.46	122.45
26	1	2030	6MZ	C9-N6-C6	-2.55	120.68	122.87
26	1	1835	2MG	O6-C6-C5	-2.53	119.88	126.60
26	1	745	1MG	C8-N7-C5	2.51	108.78	104.24
29	5	54	5MU	O4-C4-N3	-2.50	115.32	120.12
26	1	1835	2MG	N9-C8-N7	-2.48	108.72	113.39
27	2	1516	2MG	N9-C4-N3	2.48	130.92	125.94
26	1	2445	2MG	N9-C8-N7	-2.48	108.72	113.39
27	2	1207	2MG	C1'-N9-C4	-2.47	119.17	126.50
26	1	2030	6MZ	C6-C5-N7	2.47	135.06	132.39
26	1	2445	2MG	O6-C6-C5	-2.45	120.10	126.60
26	1	2251	OMG	C5-C6-N1	2.43	119.37	113.19
29	5	55	PSU	C6-N1-C2	-2.42	120.21	122.68
26	1	2580	PSU	O4'-C1'-C2'	2.42	108.56	105.14
26	1	2503	2MA	CM2-C2-N1	2.41	120.92	117.15
26	1	2552	OMU	CM2-O2'-C2'	-2.41	108.21	114.52
27	2	1207	2MG	O6-C6-C5	-2.40	120.24	126.60
26	1	1835	2MG	N1-C2-N3	-2.39	120.26	123.95
26	1	2445	2MG	CM2-N2-C2	-2.36	118.64	123.86
27	2	966	2MG	N9-C8-N7	-2.36	108.95	113.39
26	1	2503	2MA	C4-N9-C8	2.35	108.27	105.73
26	1	2069	G7M	N9-C8-N7	-2.34	106.41	112.21
26	1	2580	PSU	C6-N1-C2	-2.33	120.30	122.68
26	1	1939	5MU	C6-N1-C2	-2.33	118.94	121.30
26	1	746	PSU	O2-C2-N1	-2.32	120.24	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1	745	1MG	O6-C6-C5	-2.32	118.56	124.70
29	5	20	H2U	O2-C2-N1	-2.31	120.20	123.11
27	2	967	5MC	CM5-C5-C6	-2.31	119.76	122.85
26	1	2251	OMG	C2-N1-C6	-2.31	120.89	125.10
26	1	2503	2MA	C5-C6-N6	-2.30	118.42	123.43
27	2	1498	UR3	C3U-N3-C4	2.30	121.18	117.89
29	5	55	PSU	C6-C5-C4	2.30	119.80	118.20
26	1	1618	6MZ	C5-C6-N1	2.29	120.64	118.20
46	q	89	0TD	OD1-CG-CB	-2.28	117.66	122.44
27	2	966	2MG	N1-C2-N3	-2.28	120.42	123.95
26	1	2503	2MA	C6-C5-C4	2.27	120.23	117.18
27	2	1207	2MG	N1-C2-N3	-2.26	120.46	123.95
29	5	32	4OC	C6-C5-C4	2.25	119.71	116.96
26	1	2605	PSU	O2-C2-N3	-2.23	117.61	121.82
26	1	2504	PSU	C5-C4-N3	2.22	121.61	116.58
26	1	2251	OMG	C8-N7-C5	2.22	108.26	104.24
26	1	2457	PSU	C6-C5-C4	2.22	119.75	118.20
26	1	747	5MU	C5M-C5-C6	-2.21	119.90	122.85
29	5	54	5MU	C1'-N1-C2	2.21	121.56	117.57
26	1	746	PSU	C6-N1-C2	-2.20	120.43	122.68
27	2	1207	2MG	C8-N7-C5	2.20	108.22	104.24
26	1	1911	PSU	C6-N1-C2	-2.19	120.45	122.68
26	1	1618	6MZ	C9-N6-C6	-2.16	121.01	122.87
26	1	1915	3TD	C6-C5-C4	2.16	119.71	118.22
26	1	1917	PSU	C6-N1-C2	-2.15	120.48	122.68
26	1	2251	OMG	C4-C5-N7	-2.14	107.33	110.72
26	1	1911	PSU	O2-C2-N1	-2.10	120.48	122.79
26	1	1835	2MG	CM2-N2-C2	-2.09	119.24	123.86
27	2	1516	2MG	C1'-N9-C4	-2.09	120.30	126.50
26	1	2251	OMG	C6-C5-N7	2.08	134.12	130.25
26	1	955	PSU	C6-N1-C2	-2.07	120.56	122.68
27	2	516	PSU	C5-C4-N3	2.05	121.23	116.58
27	2	527	7MG	C6-C5-C4	-2.04	118.41	122.62
27	2	1207	2MG	C4-C5-N7	-2.04	107.49	110.72
27	2	1207	2MG	C1'-N9-C8	2.02	132.46	126.70
26	1	2605	PSU	C5-C4-N3	2.00	121.11	116.58

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	2	516	PSU	O4'-C1'-C5-C4

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Mol	Chain	Res	Type	Atoms
27	2	516	PSU	O4'-C1'-C5-C6
29	5	20	H2U	O4'-C1'-N1-C6
46	q	89	0TD	CG-CB-SB-CSB
26	1	746	PSU	C2'-C1'-C5-C4
26	1	1915	3TD	O4'-C1'-C5-C4
26	1	1915	3TD	C2'-C1'-C5-C6
26	1	1915	3TD	O4'-C1'-C5-C6
26	1	1915	3TD	C3'-C4'-C5'-O5'
26	1	1915	3TD	O4'-C4'-C5'-O5'
26	1	2251	OMG	C1'-C2'-O2'-CM2
26	1	2445	2MG	C3'-C4'-C5'-O5'
26	1	2030	6MZ	O4'-C4'-C5'-O5'
26	1	2030	6MZ	C3'-C4'-C5'-O5'
29	5	76	8AN	C3'-C4'-C5'-O5'
29	5	54	5MU	C3'-C4'-C5'-O5'
29	5	54	5MU	O4'-C4'-C5'-O5'
26	1	1618	6MZ	O4'-C4'-C5'-O5'
26	1	1618	6MZ	C3'-C4'-C5'-O5'
29	5	76	8AN	C4'-C5'-O5'-P
29	5	20	H2U	O4'-C4'-C5'-O5'
29	5	20	H2U	C3'-C4'-C5'-O5'
26	1	2445	2MG	O4'-C4'-C5'-O5'
27	2	966	2MG	C3'-C4'-C5'-O5'
27	2	1402	4OC	O4'-C4'-C5'-O5'
29	5	76	8AN	O4'-C4'-C5'-O5'
26	1	2552	OMU	C3'-C2'-O2'-CM2
27	2	966	2MG	O4'-C4'-C5'-O5'
29	5	8	4SU	C2'-C1'-N1-C6
29	5	8	4SU	O4'-C1'-N1-C6
29	5	20	H2U	O4'-C1'-N1-C2
27	2	527	7MG	C3'-C4'-C5'-O5'
27	2	1402	4OC	C3'-C4'-C5'-O5'
27	2	527	7MG	C4'-C5'-O5'-P
26	1	746	PSU	O4'-C1'-C5-C6
29	5	8	4SU	C2'-C1'-N1-C2
26	1	2503	2MA	C4'-C5'-O5'-P
29	5	8	4SU	O4'-C1'-N1-C2
26	1	2069	G7M	O4'-C4'-C5'-O5'
29	5	20	H2U	C2'-C1'-N1-C2
26	1	2503	2MA	O4'-C4'-C5'-O5'
26	1	2498	OMC	C4'-C5'-O5'-P

There are no ring outliers.

9 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	1	2503	2MA	1	0
26	1	1939	5MU	2	0
26	1	2251	OMG	1	0
27	2	1402	4OC	1	0
26	1	2069	G7M	1	0
27	2	1516	2MG	1	0
29	5	32	4OC	2	0
27	2	1519	MA6	1	0
26	1	2030	6MZ	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 440 ligands modelled in this entry, 439 are monoatomic - leaving 1 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	$\# Z > 2$
59	FME	5	104	29	8,9,10	0.88	0	7,9,11	1.82	1 (14%)

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
59	FME	5	104	29	-	4/7/9/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	5	104	FME	CA-N-CN	4.05	129.05	122.82

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	5	104	FME	CB-CA-N-CN
59	5	104	FME	N-CA-CB-CG
59	5	104	FME	CB-CG-SD-CE
59	5	104	FME	CA-CB-CG-SD

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	5	104	FME	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
27	2	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	147:G	O3'	148:G	P	3.01
1	2	1276:G	O3'	1277:C	P	2.98

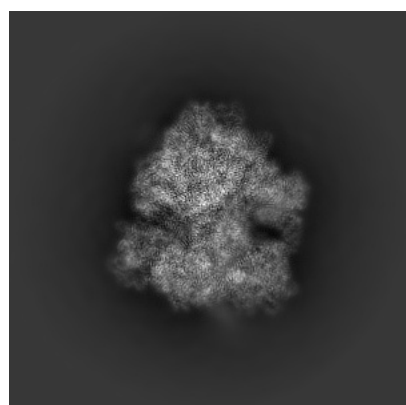
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12635. These allow visual inspection of the internal detail of the map and identification of artifacts.

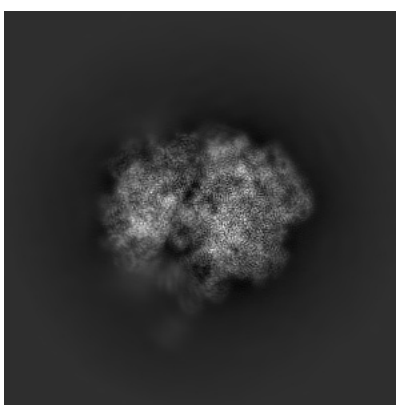
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

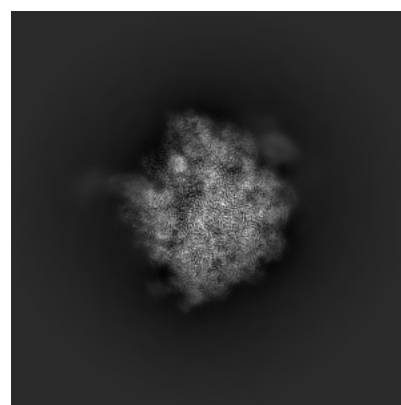
6.1.1 Primary map



X



Y

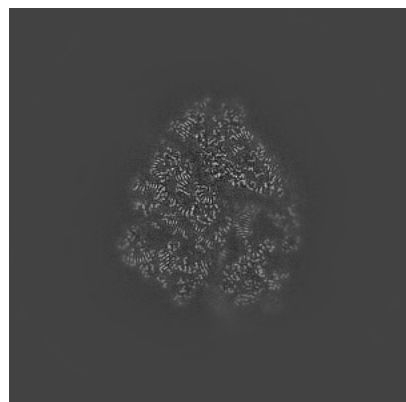


Z

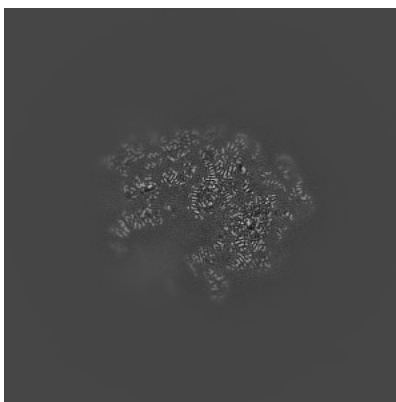
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

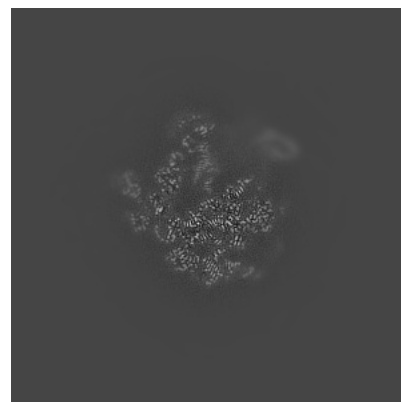
6.2.1 Primary map



X Index: 225



Y Index: 225

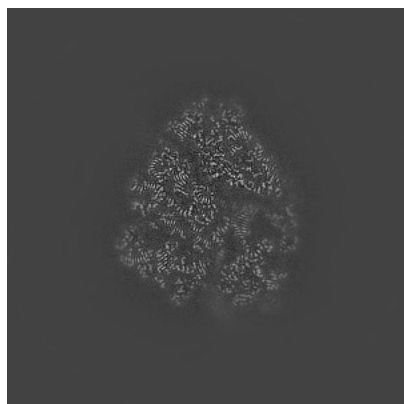


Z Index: 225

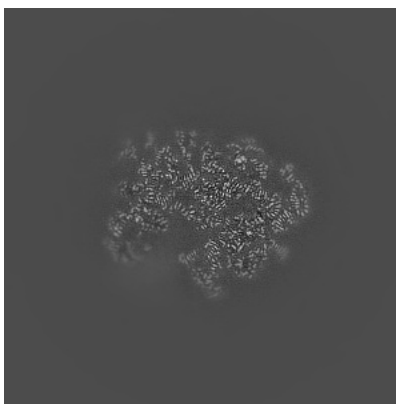
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

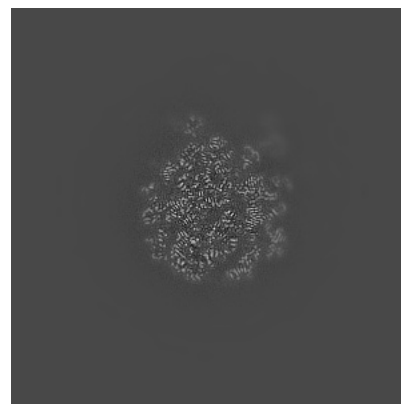
6.3.1 Primary map



X Index: 225



Y Index: 215

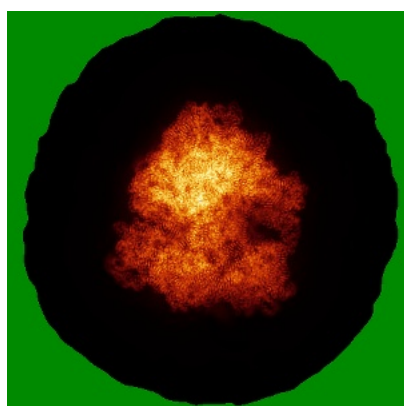


Z Index: 264

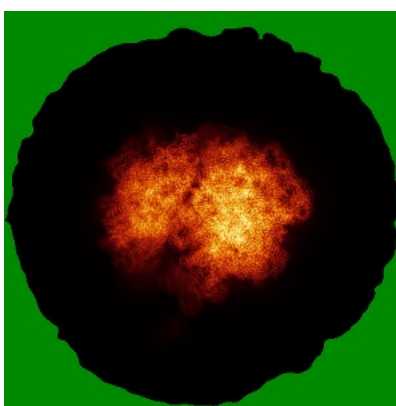
The images above show the largest variance slices of the map in three orthogonal directions.

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

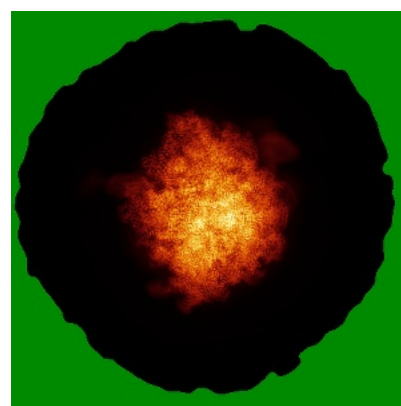
6.4.1 Primary map



X



Y

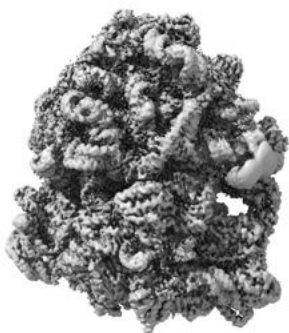


Z

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 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

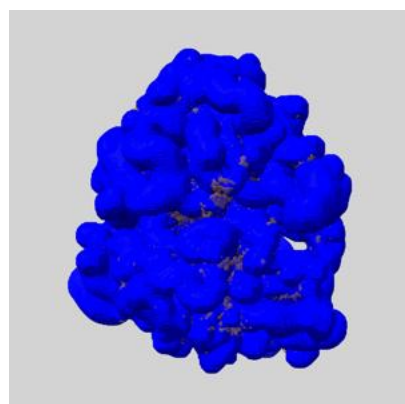
6.6 Mask visualisation [i](#)

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

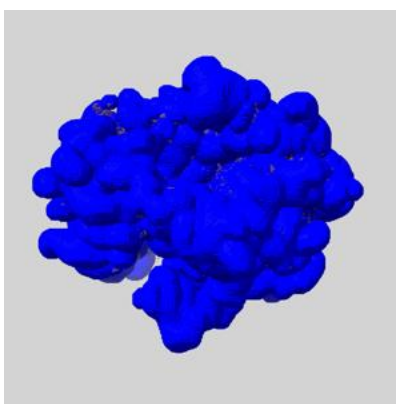
A mask typically either:

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

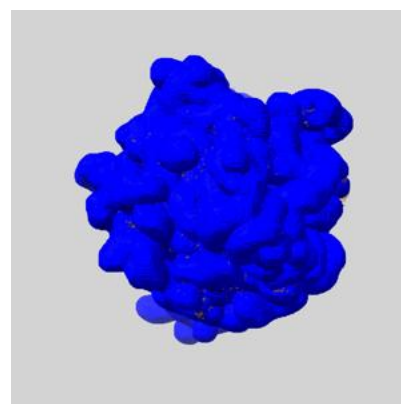
6.6.1 emd_12635_msk_1.map [i](#)



X



Y

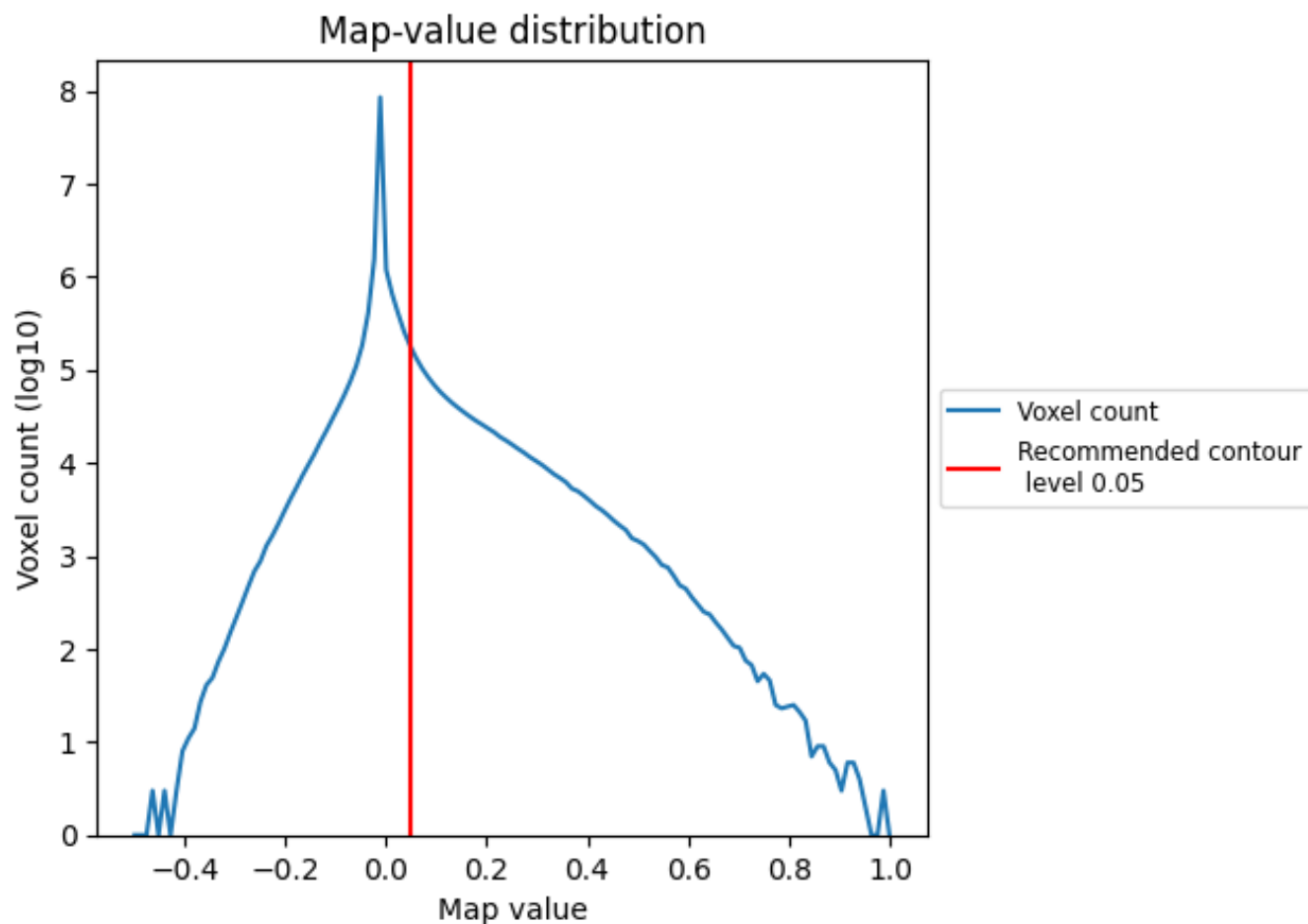


Z

7 Map analysis [i](#)

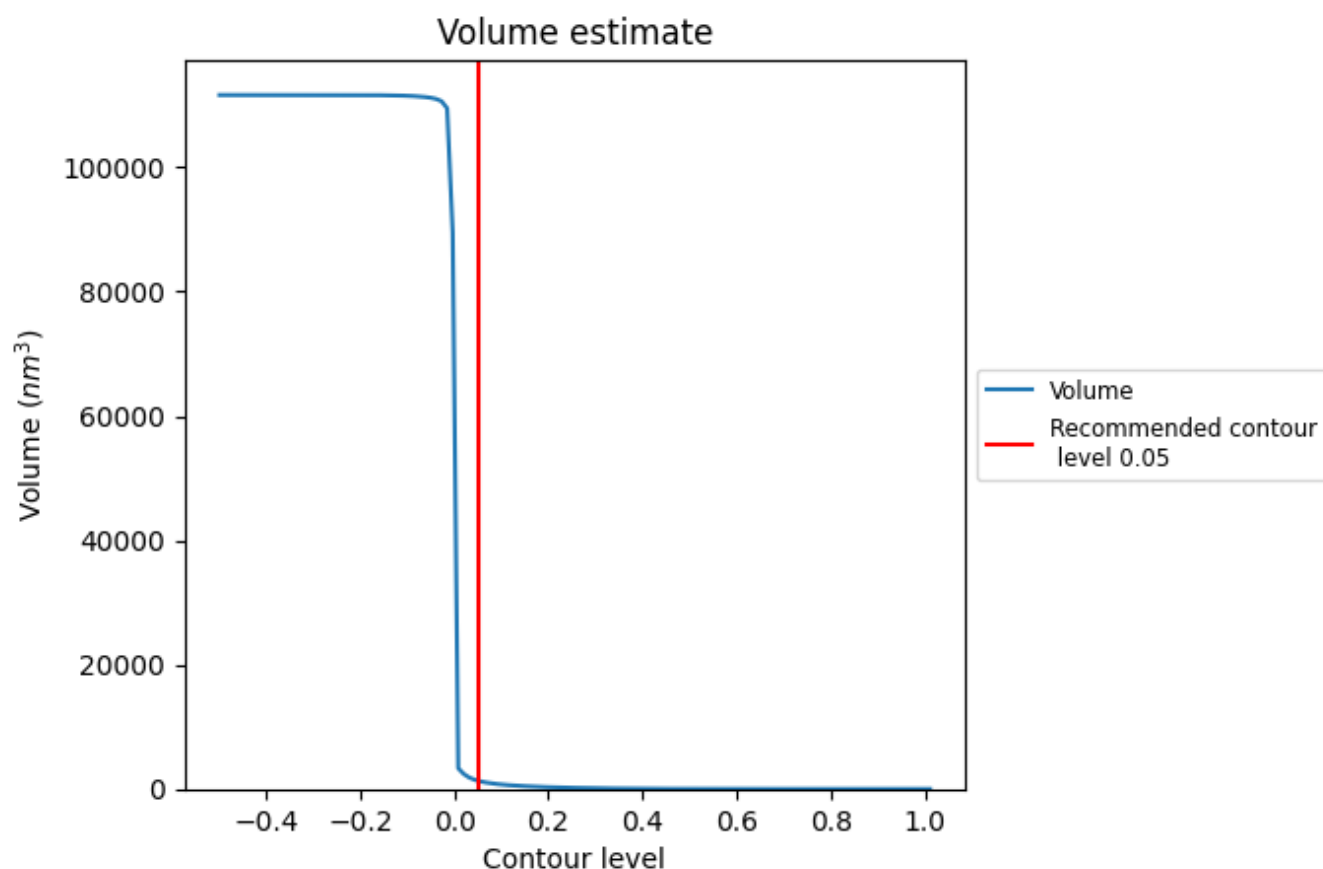
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

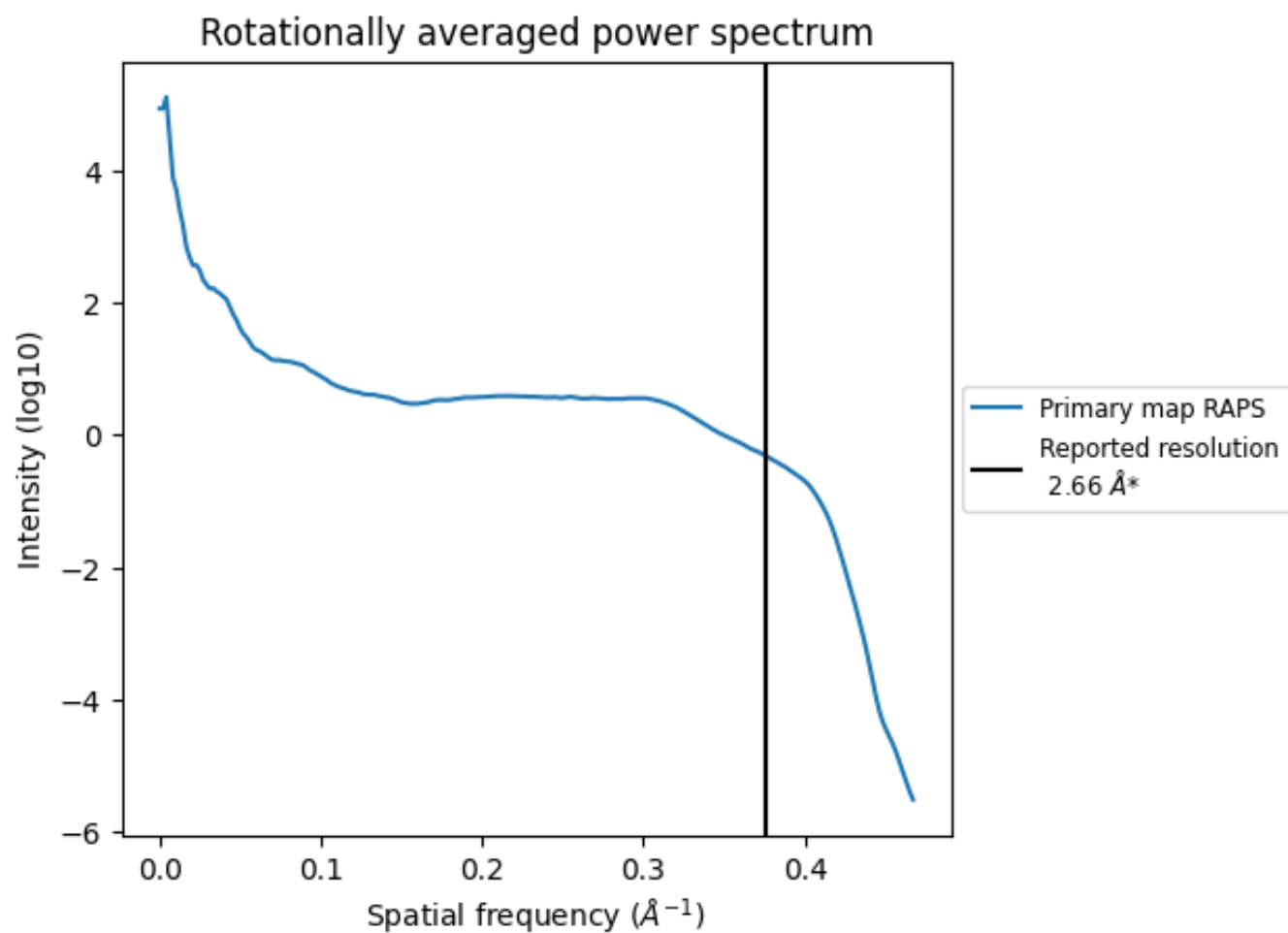
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1344 nm^3 ; this corresponds to an approximate mass of 1214 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 ⓘ

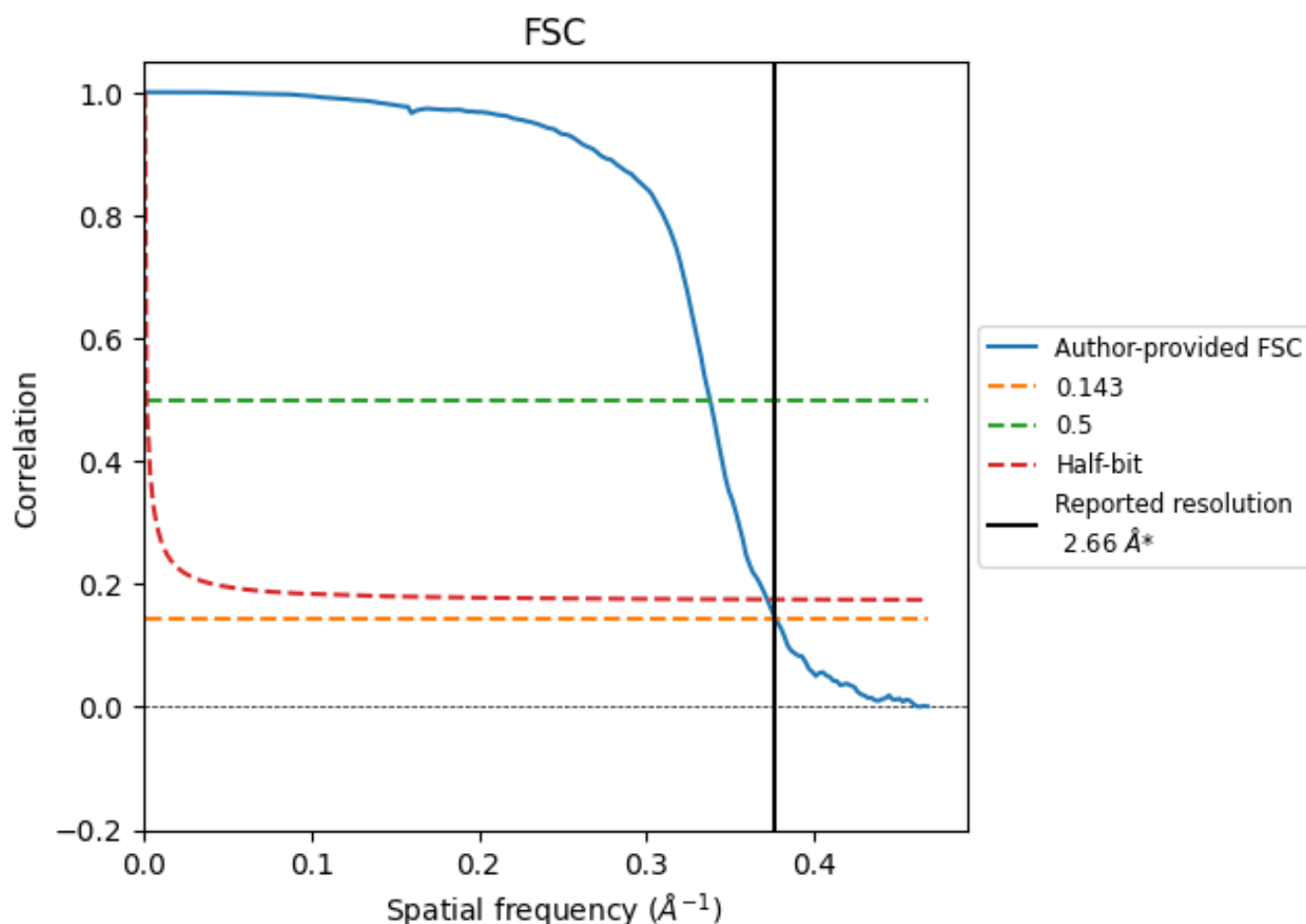


*Reported resolution corresponds to spatial frequency of 0.376 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.376 Å⁻¹

8.2 Resolution estimates [i](#)

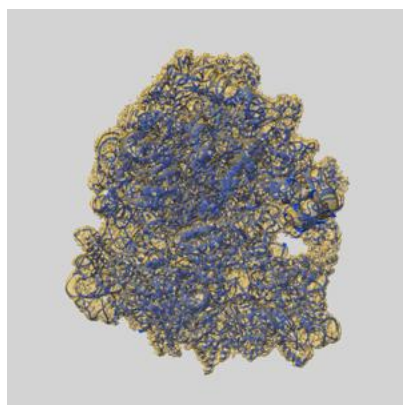
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.66	-	-
Author-provided FSC curve	2.65	2.96	2.69
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

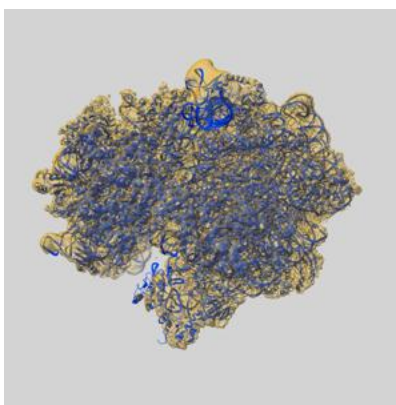
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12635 and PDB model 7NWT. Per-residue inclusion information can be found in section [3](#) on page [17](#).

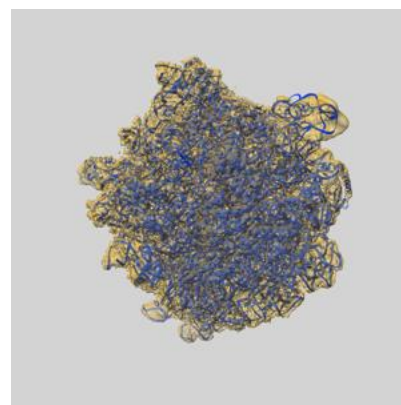
9.1 Map-model overlay [i](#)



X



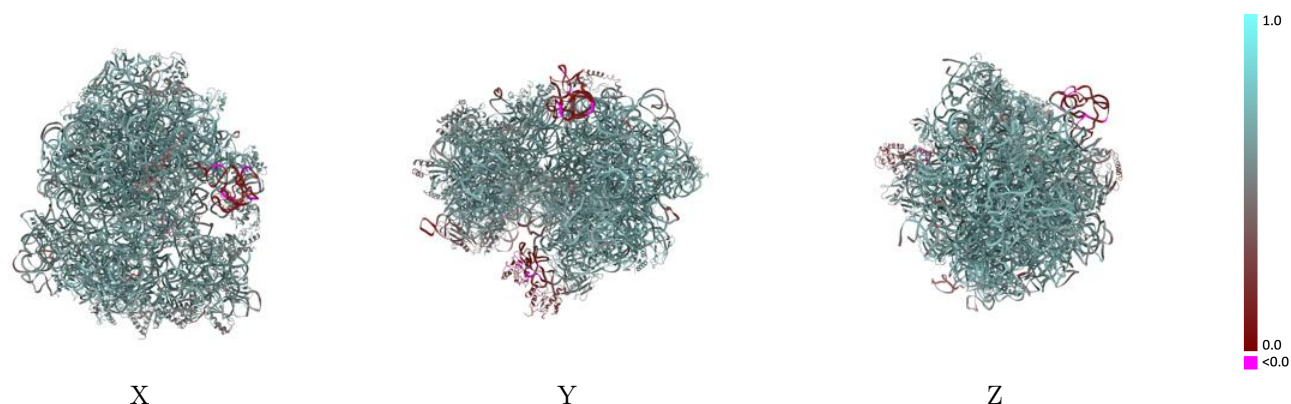
Y



Z

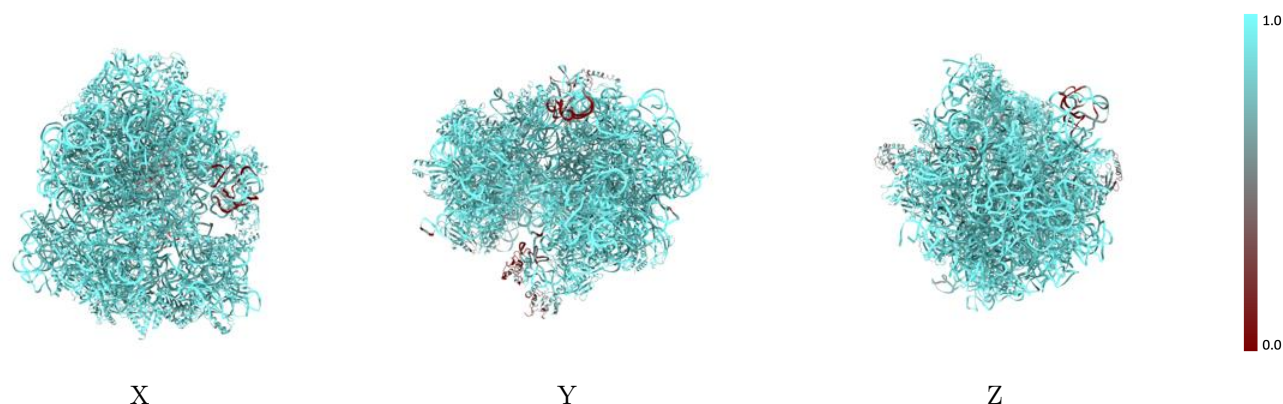
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



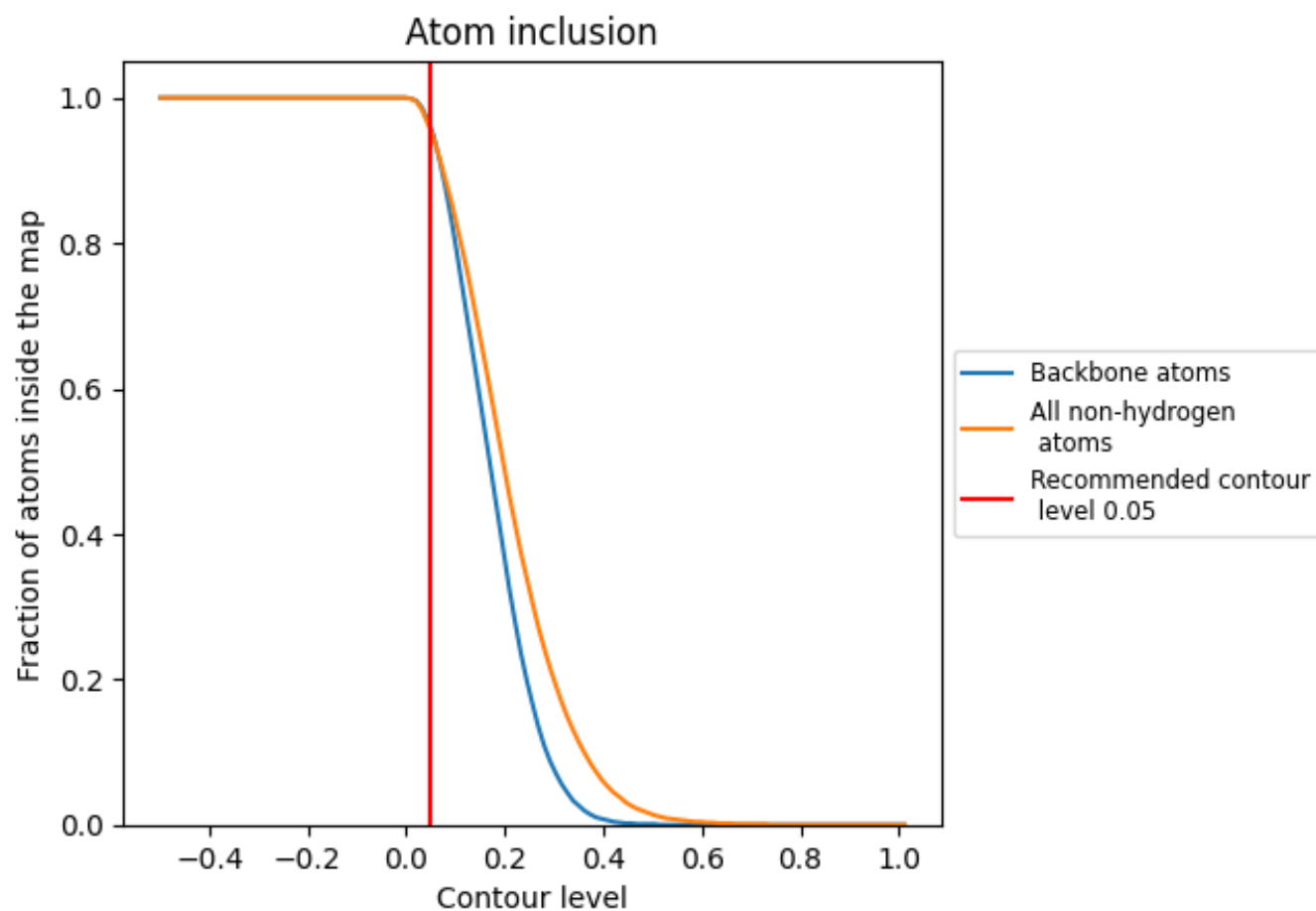
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9550	 0.6140
1	 0.9720	 0.6290
2	 0.9880	 0.6210
3	 0.9930	 0.6160
5	 0.9470	 0.5870
AA	 0.8730	 0.4670
B	 0.9860	 0.6810
BB	 0.8910	 0.5400
C	 0.9720	 0.6640
CC	 0.7050	 0.4130
D	 0.9630	 0.6350
E	 0.9210	 0.5760
F	 0.9180	 0.5590
G	 0.6550	 0.4570
H	 0.5480	 0.1950
I	 0.2570	 0.1390
J	 0.9730	 0.6590
K	 0.9710	 0.6640
L	 0.9730	 0.6570
M	 0.9650	 0.6500
N	 0.9910	 0.6780
O	 0.9530	 0.6090
P	 0.9620	 0.6570
Q	 0.9860	 0.6770
R	 0.9590	 0.6400
S	 0.9640	 0.6590
T	 0.9510	 0.6390
U	 0.9550	 0.6110
V	 0.9360	 0.6110
W	 0.9700	 0.6670
X	 0.9700	 0.6630
XX	 0.9720	 0.5960
Y	 0.9320	 0.5850
Z	 0.9680	 0.6460
a	 0.8400	 0.4930



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Chain	Atom inclusion	Q-score
b	 0.9600	 0.6600
c	 0.9400	 0.6330
d	 0.9830	 0.6980
e	 0.9880	 0.6850
f	 0.9830	 0.6520
g	 0.9030	 0.5490
h	 0.9260	 0.5950
i	 0.9500	 0.6120
j	 0.9660	 0.6410
k	 0.9360	 0.5860
l	 0.9070	 0.5700
m	 0.9670	 0.6320
n	 0.9480	 0.5840
o	 0.9070	 0.5440
p	 0.9460	 0.6100
q	 0.9520	 0.6450
r	 0.9330	 0.5890
s	 0.9640	 0.6180
t	 0.9550	 0.6200
u	 0.9540	 0.6300
v	 0.9420	 0.6000
w	 0.9310	 0.6130
x	 0.9430	 0.5800
y	 0.9600	 0.6210
z	 0.8100	 0.5550