Full wwPDB EM Validation Report ⓘ

Sep 28, 2024 – 09:32 pm BST

PDB ID	:	6SWC
EMDB ID	:	EMD-10322
Title	:	IC2B model of cryo-EM structure of a full archaeal ribosomal translation initiation complex devoid of aIF1 in P. abyssi
Authors	:	Coureux, P.-D.; Mechulam, Y.; Schmitt, E.
Deposited on	:	2019-09-20
Resolution	:	3.30 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

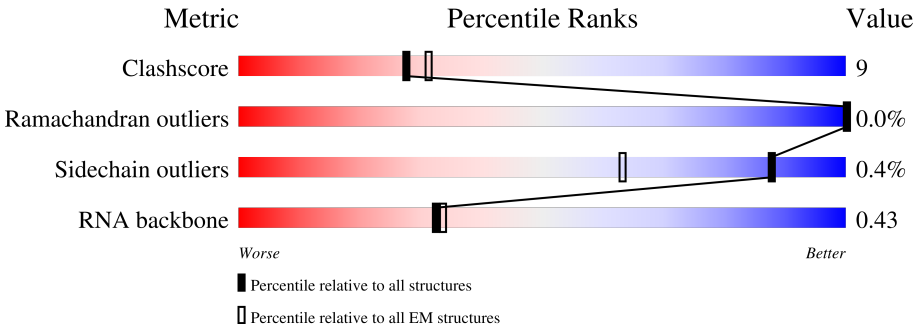
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	2	1497	63% 29% 8%
2	A	199	73% 22% 6%
3	B	202	80% 17% .
4	C	63	78% 19% .
5	D	180	86% 11% . .
6	E	243	79% 20%
7	F	236	80% 17% .

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Mol	Chain	Length	Quality of chain
8	G	125	68% 31%
9	H	215	79% 20%
10	I	130	76% 23%
11	J	127	79% 20%
12	K	135	81% 19%
13	L	102	80% 19%
14	M	137	78% 15% 7%
15	N	147	80% 20%
16	O	148	73% 24%
17	P	56	82% 16%
18	Q	158	73% 23%
19	R	113	80% 16%
20	S	67	72% 27%
21	T	132	73% 24%
22	U	150	83% 16%
23	V	99	73% 22% 5%
24	W	65	62% 35%
25	X	71	75% 18% 6%
26	Y	51	61% 31% 6%
27	Z	210	78% 16% 6%
28	0	36	75% 25%
29	3	123	37% 63%
30	5	20	60% 30% 10%
31	4	76	20% 43% 34%
32	6	113	43% 41% 16%

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Mol	Chain	Length	Quality of chain
33	7	415	
34	8	139	
35	9	266	

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 70744 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	1497	32291	14394	5959	10441	1497	0	0

- Molecule 2 is a protein called 30S ribosomal protein S3Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	188	1533	995	268	266	4	0	0

- Molecule 3 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	196	1571	1017	269	281	4	0	0

- Molecule 4 is a protein called Zn-ribbon RNA-binding protein involved in translation.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	61	482	304	85	85	8	0	0

- Molecule 5 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	D	175	1470	924	284	258	4	0	0

- Molecule 6 is a protein called 30S ribosomal protein S4e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	E	242	1983	1281	358	339	5	0	0

- Molecule 7 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	229	Total	C	N	O	S	0	0
			1808	1147	334	320	7		

- Molecule 8 is a protein called 30S ribosomal protein S6e.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	124	Total	C	N	O	S	0	0
			977	621	178	176	2		

- Molecule 9 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	213	Total	C	N	O	S	0	0
			1720	1092	322	299	7		

- Molecule 10 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	129	Total	C	N	O	S	0	0
			1034	668	184	180	2		

- Molecule 11 is a protein called 30S ribosomal protein S8e.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	J	126	Total	C	N	O	0	0
			996	617	206	173		

- Molecule 12 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	134	Total	C	N	O	S	0	0
			1065	668	206	188	3		

- Molecule 13 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	101	Total	C	N	O	S	0	0
			817	507	158	148	4		

- Molecule 14 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	128	Total	C	N	O	S	0	0
			964	597	192	173	2		

- Molecule 15 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	146	Total	C	N	O	S	0	0
			1148	727	224	194	3		

- Molecule 16 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	143	Total	C	N	O	S	0	0
			1151	721	229	196	5		

- Molecule 17 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	55	Total	C	N	O	S	0	0
			455	288	95	67	5		

- Molecule 18 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	152	Total	C	N	O	S	0	0
			1262	804	240	214	4		

- Molecule 19 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	109	Total	C	N	O	S	0	0
			900	572	174	151	3		

- Molecule 20 is a protein called 30S ribosomal protein S17e.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	66	Total	C	N	O	S	0	0
			558	355	106	96	1		

- Molecule 21 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	130	Total	C	N	O	S	0	0
			1057	675	201	174	7		

- Molecule 22 is a protein called 30S ribosomal protein S19e.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	U	149	Total	C	N	O	0	0
			1223	790	221	212		

- Molecule 23 is a protein called 30S ribosomal protein S24e.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	94	Total	C	N	O	S	0	0
			790	516	125	146	3		

- Molecule 24 is a protein called 30S ribosomal protein S27e.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	63	Total	C	N	O	S	0	0
			481	303	93	80	5		

- Molecule 25 is a protein called 30S ribosomal protein S28e.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	X	67	Total	C	N	O	0	0
			536	327	111	98		

- Molecule 26 is a protein called 30S ribosomal protein S27ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	50	Total	C	N	O	S	0	0
			408	262	77	63	6		

- Molecule 27 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	197	Total	C	N	O	S	0	0
			1550	989	286	271	4		

- Molecule 28 is a protein called 30S ribosomal protein aL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	0	36	Total	C	N	O	S	0	0
			343	218	84	39	2		

- Molecule 29 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	3	123	Total	C	N	O	S	0	0
			941	599	157	181	4		

- Molecule 30 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	5	20	Total	C	N	O	P	0	0
			430	192	78	140	20		

- Molecule 31 is a RNA chain called initiator Met-tRNA fMet from E. coli (A1U72 variant).

Mol	Chain	Residues	Atoms						AltConf	Trace
31	4	76	Total	C	N	O	P	S	0	0
			1622	724	291	530	76	1		

- Molecule 32 is a protein called Translation initiation factor 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	6	95	Total	C	N	O	S	0	0
			777	496	148	130	3		

- Molecule 33 is a protein called Translation initiation factor 2 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	7	414	Total	C	N	O	S	0	0
			3213	2058	548	595	12		

- Molecule 34 is a protein called Translation initiation factor 2 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	8	129	Total	C	N	O	S	0	0
			1033	659	172	192	10		

- Molecule 35 is a protein called Translation initiation factor 2 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	9	254	Total	C	N	O	S	0	0
			2033	1301	346	384	2		

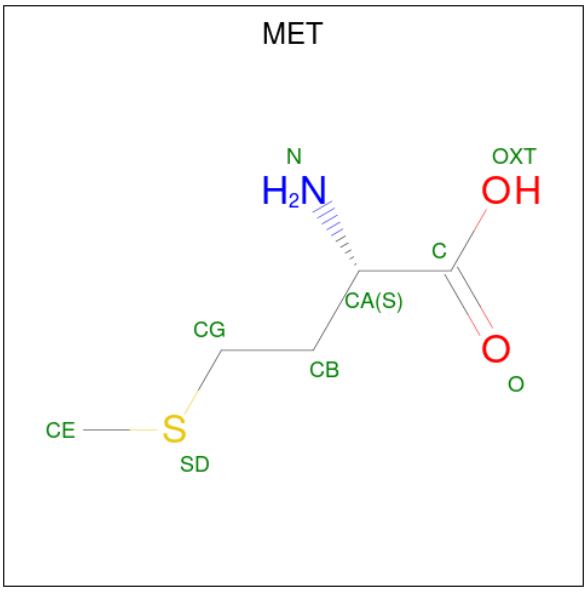
- Molecule 36 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
36	2	30	Total	Mg	0
			30	30	
36	5	2	Total	Mg	0
			2	2	
36	4	1	Total	Mg	0
			1	1	
36	7	1	Total	Mg	0
			1	1	

- Molecule 37 is ZINC ION (three-letter code: ZN) (formula: Zn).

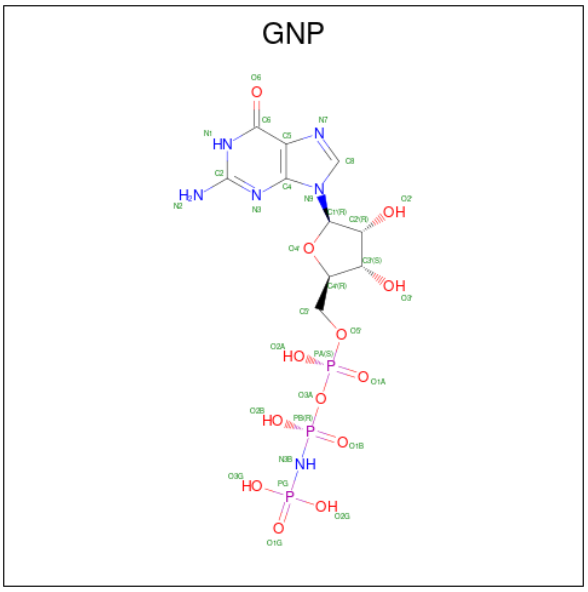
Mol	Chain	Residues	Atoms		AltConf
37	C	2	Total	Zn	0
			2	2	
37	F	1	Total	Zn	0
			1	1	
37	P	1	Total	Zn	0
			1	1	
37	R	1	Total	Zn	0
			1	1	
37	W	1	Total	Zn	0
			1	1	

- Molecule 38 is METHIONINE (three-letter code: MET) (formula: $C_5H_{11}NO_2S$).



Mol	Chain	Residues	Atoms					AltConf
38	4	1	Total	C	N	O	S	0
			8	5	1	1	1	

- Molecule 39 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
39	7	1	Total	C	N	O	P	0
			32	10	6	13	3	

- Molecule 40 is water.

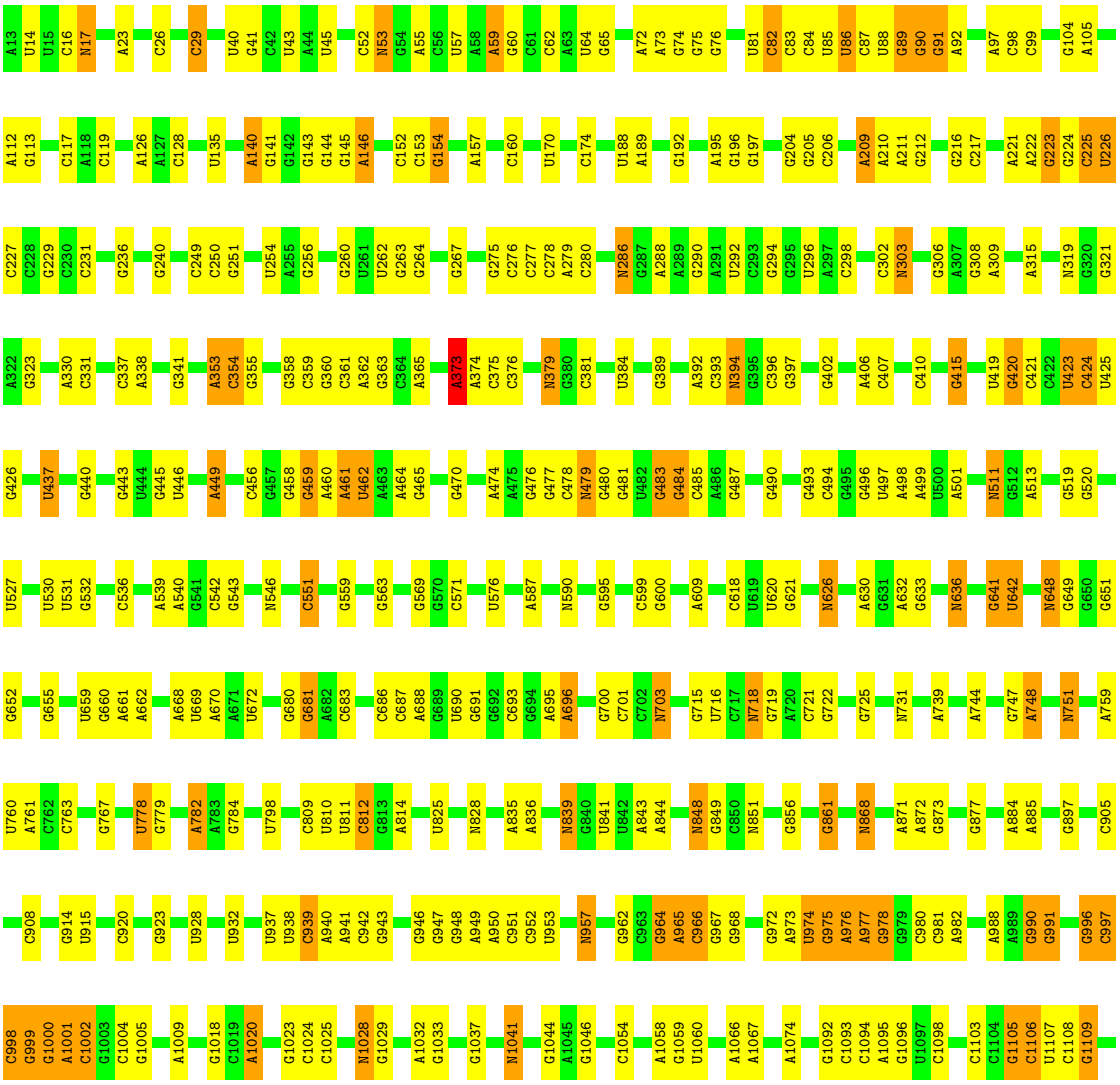
Mol	Chain	Residues	Atoms	AltConf
40	2	39	Total O 39 39	0
40	K	1	Total O 1 1	0
40	Q	1	Total O 1 1	0
40	U	1	Total O 1 1	0

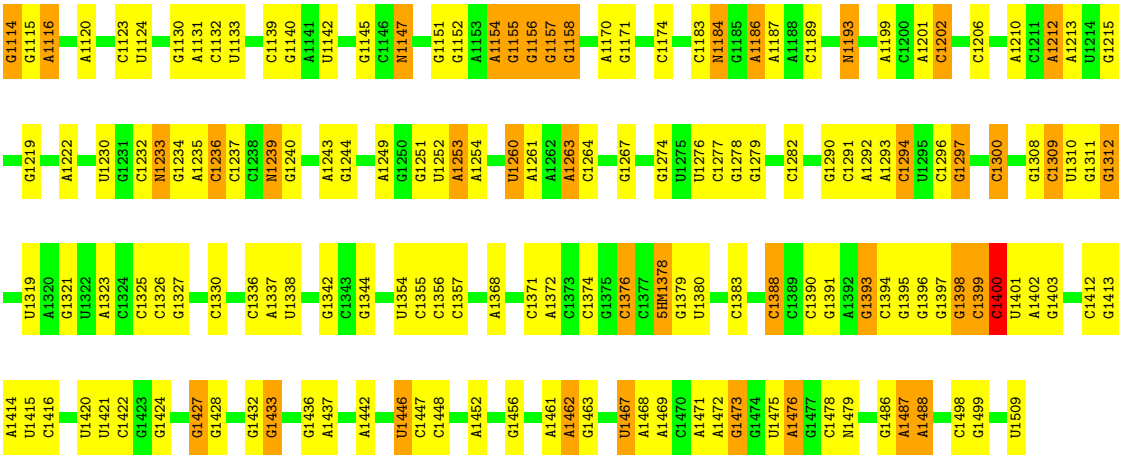
3 Residue-property plots (i)

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

- Molecule 1: 16S ribosomal rRNA

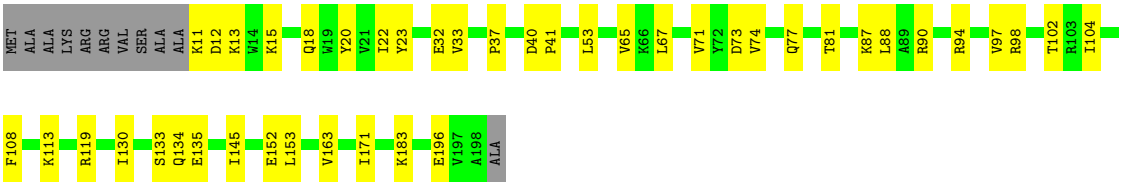
Chain 2:





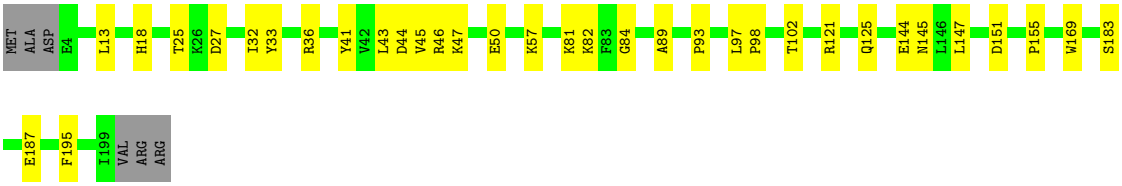
• Molecule 2: 30S ribosomal protein S3Ae

Chain A:



• Molecule 3: 30S ribosomal protein S2

Chain B:

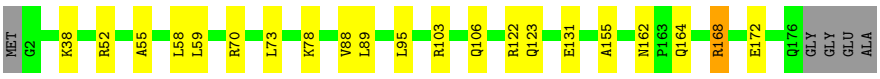


• Molecule 4: Zn-ribbon RNA-binding protein involved in translation

Chain C:

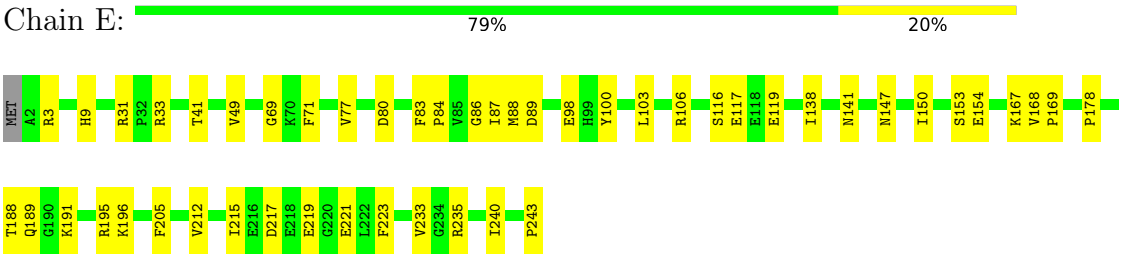
• Molecule 5: 30S ribosomal protein S4

Chain D:



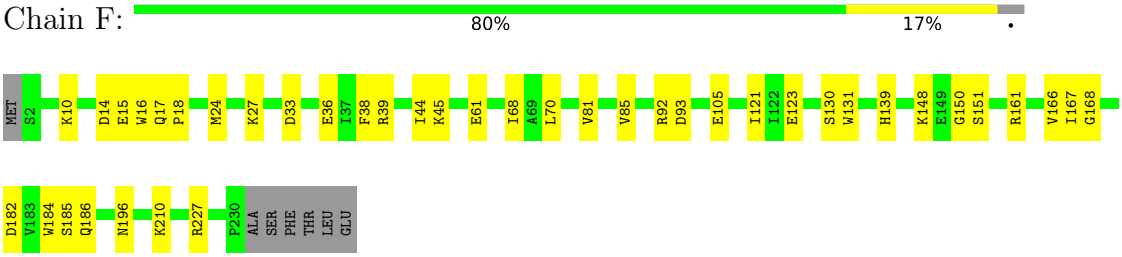
• Molecule 6: 30S ribosomal protein S4e

Chain E:



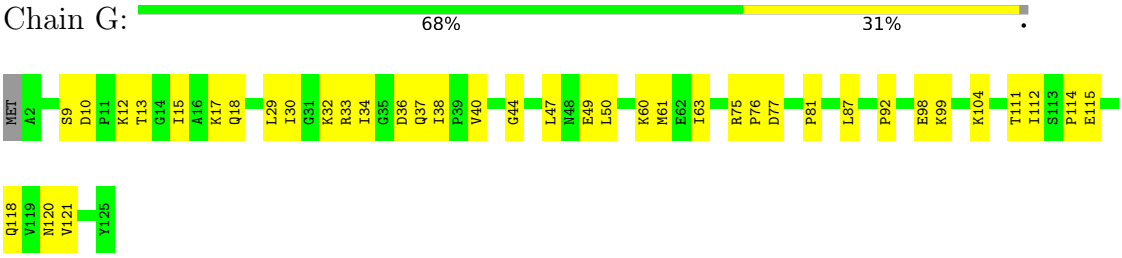
• Molecule 7: 30S ribosomal protein S5

Chain F:



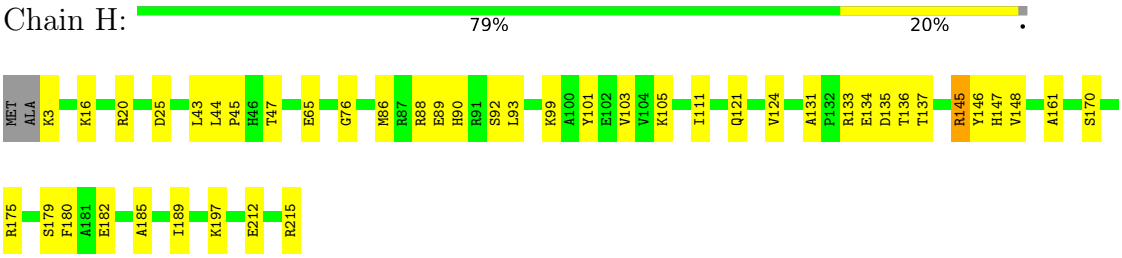
• Molecule 8: 30S ribosomal protein S6e

Chain G:



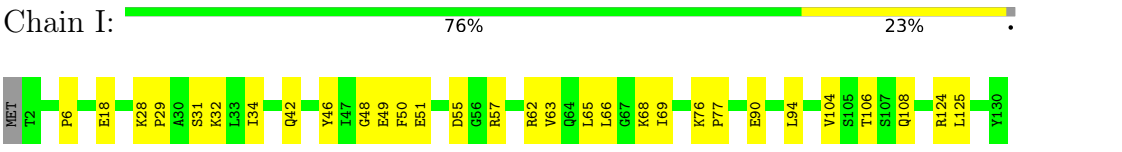
• Molecule 9: 30S ribosomal protein S7

Chain H:



• Molecule 10: 30S ribosomal protein S8

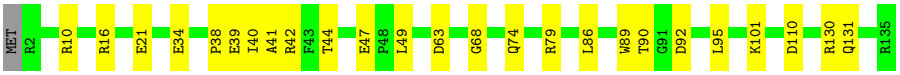
Chain I:



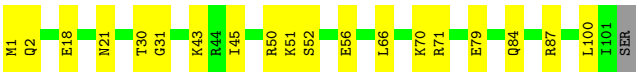
• Molecule 11: 30S ribosomal protein S8e

Chain J:

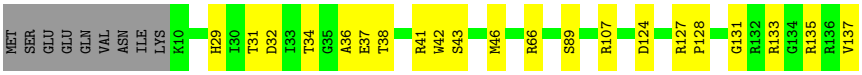
• Molecule 12: 30S ribosomal protein S9



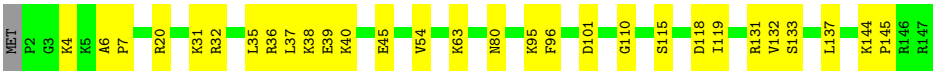
• Molecule 13: 30S ribosomal protein S10



• Molecule 14: 30S ribosomal protein S11



• Molecule 15: 30S ribosomal protein S12

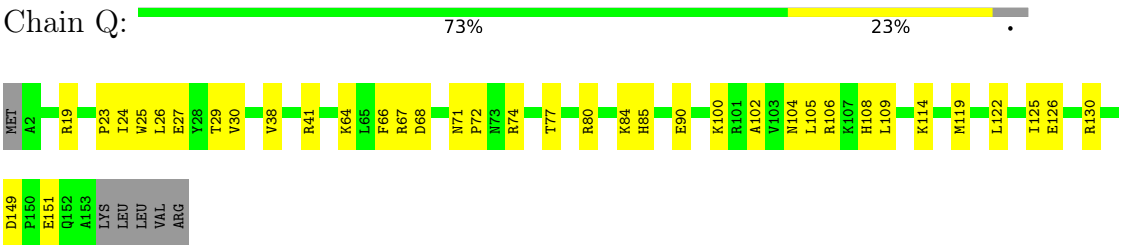


• Molecule 16: 30S ribosomal protein S13

• Molecule 17: 30S ribosomal protein S14 type Z

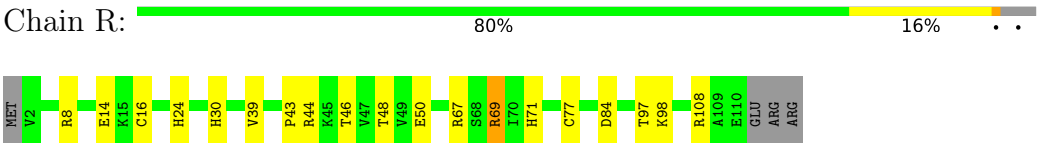
• Molecule 18: 30S ribosomal protein S15

Chain Q:



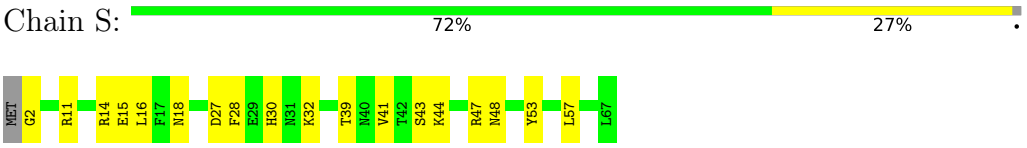
• Molecule 19: 30S ribosomal protein S17

Chain R:



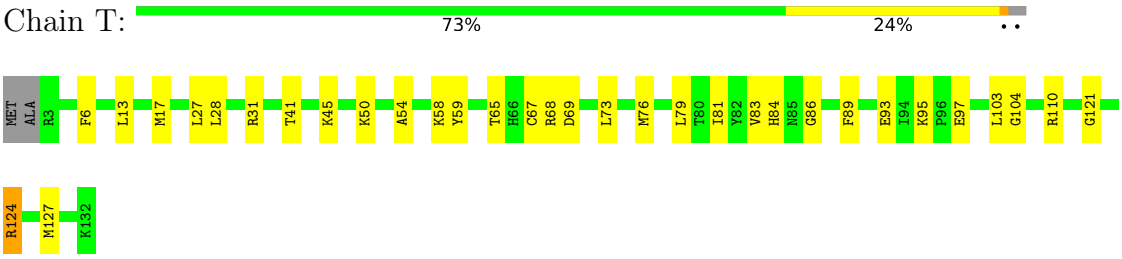
• Molecule 20: 30S ribosomal protein S17e

Chain S:



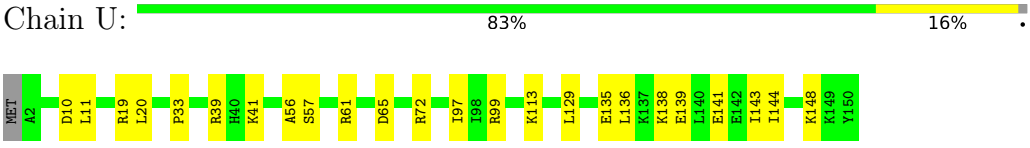
• Molecule 21: 30S ribosomal protein S19

Chain T:



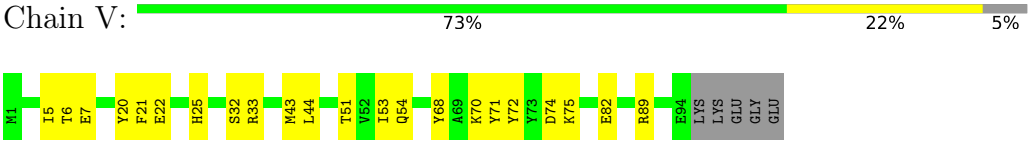
• Molecule 22: 30S ribosomal protein S19e

Chain U:



• Molecule 23: 30S ribosomal protein S24e

Chain V:



• Molecule 24: 30S ribosomal protein S27e

Chain W:

• Molecule 25: 30S ribosomal protein S28e

Chain X:

• Molecule 26: 30S ribosomal protein S27ae

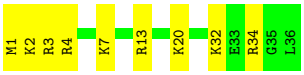
Chain Y:

• Molecule 27: 30S ribosomal protein S3

Chain Z:

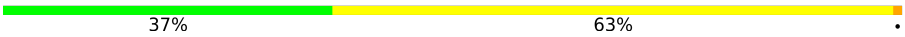
• Molecule 28: 30S ribosomal protein aL41

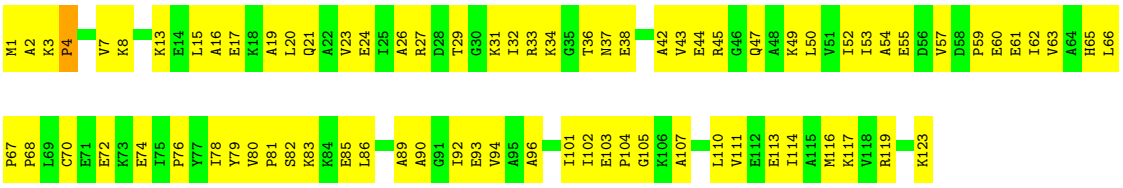
Chain 0:



• Molecule 29: 50S ribosomal protein L7Ae

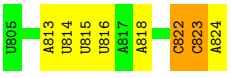
Chain 3:





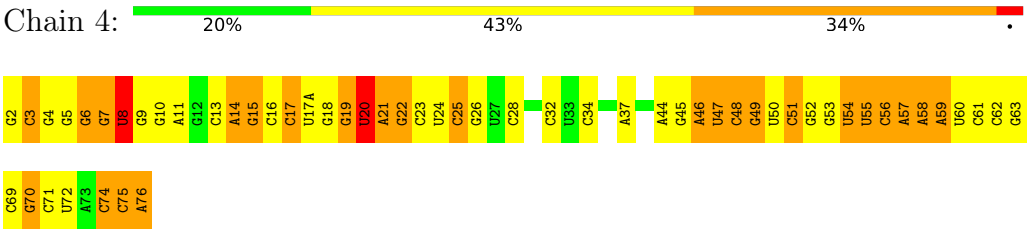
• Molecule 30: mRNA

Chain 5:



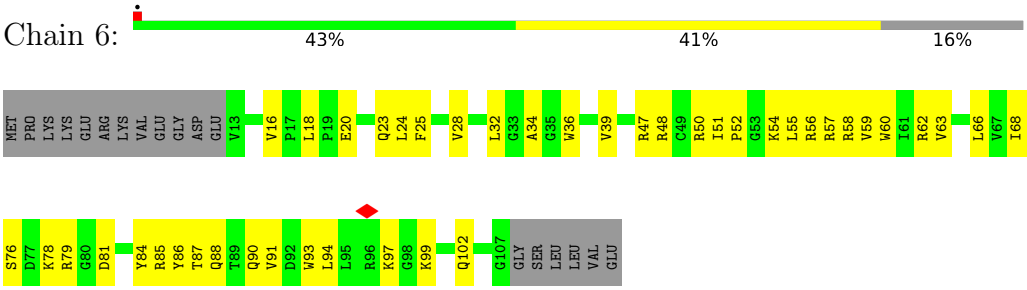
• Molecule 31: initiator Met-tRNA fMet from E. coli (A1U72 variant)

Chain 4:



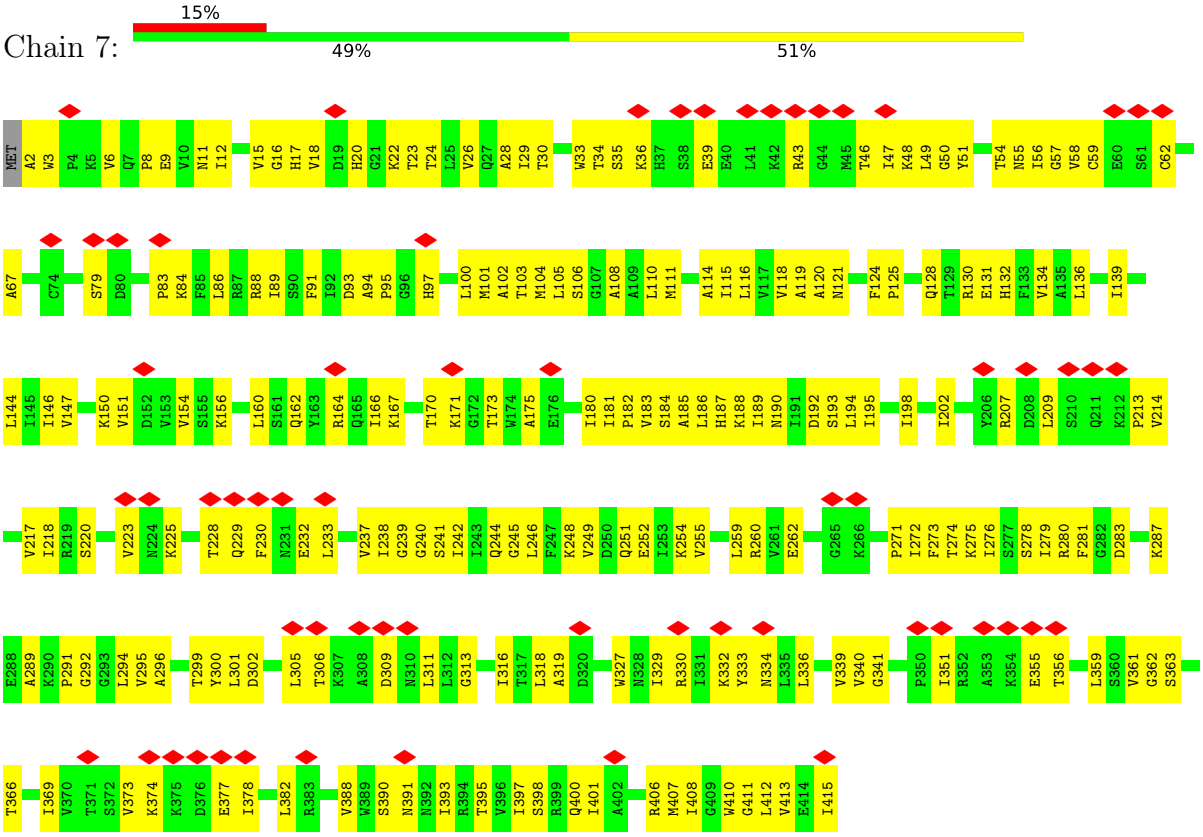
• Molecule 32: Translation initiation factor 1A

Chain 6:



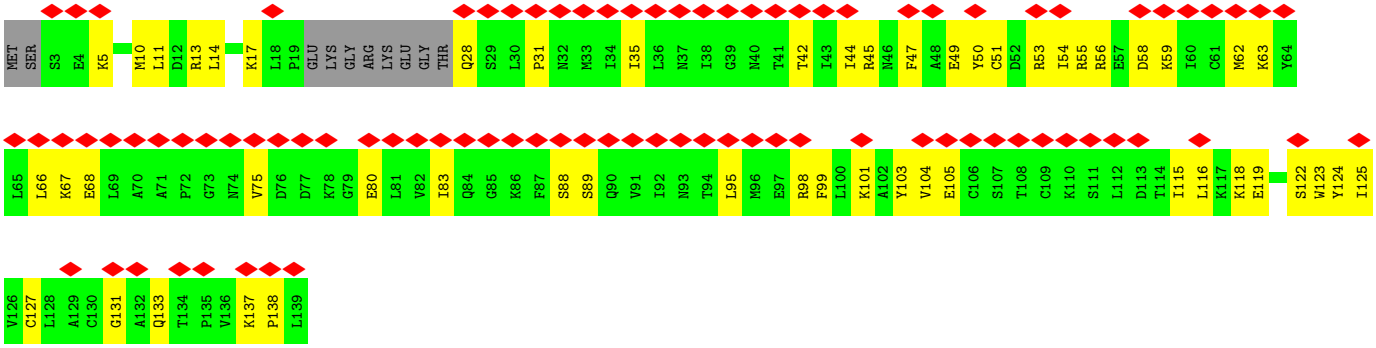
• Molecule 33: Translation initiation factor 2 subunit gamma

Chain 7:



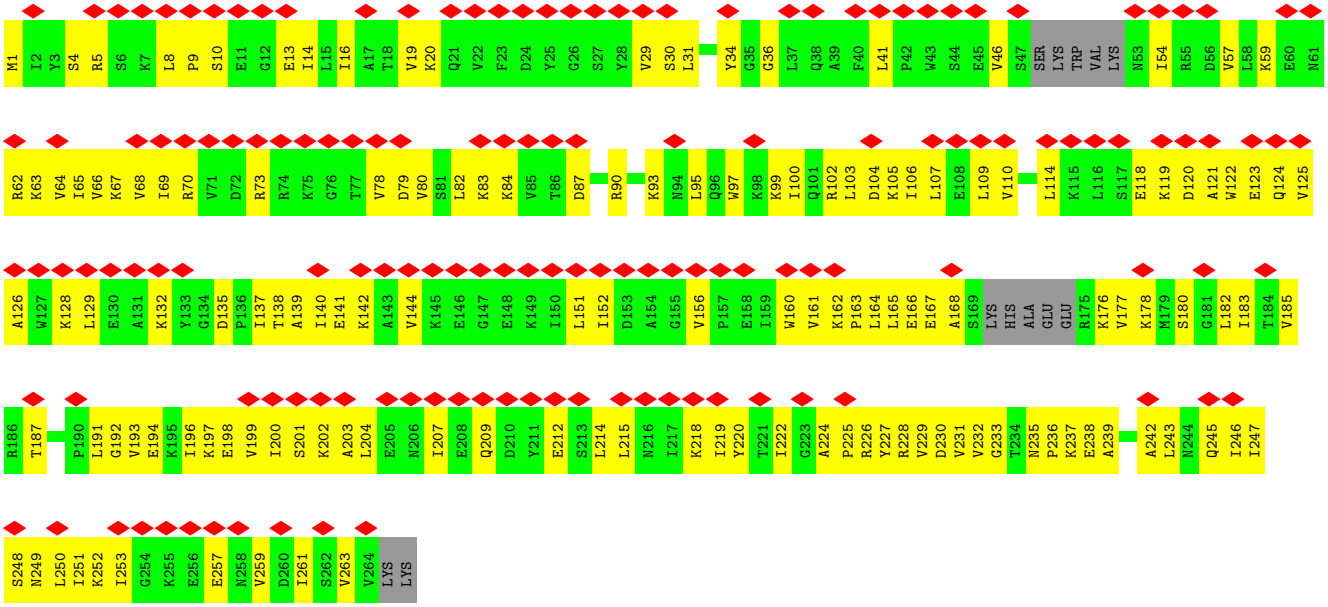
• Molecule 34: Translation initiation factor 2 subunit beta

Chain 8:



• Molecule 35: Translation initiation factor 2 subunit alpha

Chain 9:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	142000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.065	Depositor
Minimum map value	-0.017	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.003	Depositor
Map size (Å)	379.32, 379.32, 379.32	wwPDB
Map dimensions	348, 348, 348	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: B8H, GNP, 4SU, UR3, PSU, H2U, A2M, 4AC, 5MU, MG, LHH, MA6, 6MZ, 5HM, ZN, 5MC, OMC

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	2	1.21	7/35019 (0.0%)	1.02	41/54586 (0.1%)
2	A	0.51	0/1559	0.52	0/2090
3	B	0.49	0/1602	0.53	0/2165
4	C	0.53	0/496	0.57	0/673
5	D	0.49	0/1494	0.50	0/2003
6	E	0.57	0/2032	0.54	0/2742
7	F	0.56	0/1838	0.56	0/2478
8	G	0.37	0/993	0.50	0/1329
9	H	0.48	0/1757	0.53	0/2359
10	I	0.58	0/1055	0.57	0/1415
11	J	0.45	0/1005	0.53	0/1339
12	K	0.49	0/1081	0.54	0/1449
13	L	0.42	0/825	0.49	0/1107
14	M	0.47	0/982	0.54	0/1322
15	N	0.53	0/1165	0.56	0/1547
16	O	0.47	0/1170	0.54	0/1573
17	P	0.59	0/465	0.58	0/613
18	Q	0.49	0/1290	0.52	0/1734
19	R	0.54	0/923	0.54	0/1247
20	S	0.43	0/565	0.50	1/747 (0.1%)
21	T	0.48	0/1077	0.53	0/1439
22	U	0.57	0/1253	0.53	0/1689
23	V	0.52	0/808	0.52	0/1086
24	W	0.37	0/488	0.51	0/659
25	X	0.45	0/538	0.58	0/719
26	Y	0.30	0/420	0.51	0/559
27	Z	0.46	0/1572	0.55	0/2110
28	0	0.57	0/349	0.58	0/451
29	3	0.31	0/953	0.55	0/1284
30	5	0.80	0/481	0.96	0/748
31	4	0.69	0/1699	1.08	1/2648 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	6	0.32	0/793	0.48	0/1072
33	7	0.29	0/3272	0.55	2/4430 (0.0%)
34	8	0.26	0/1046	0.52	0/1402
35	9	0.28	0/2058	0.52	0/2770
All	All	0.90	7/74123 (0.0%)	0.83	45/107584 (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
26	Y	0	1
35	9	0	1
All	All	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1046	G	C5-C4	-5.24	1.34	1.38
1	2	540	A	N9-C4	-5.15	1.34	1.37
1	2	1263	A	N9-C4	-5.08	1.34	1.37
1	2	1326	C	N1-C6	-5.08	1.34	1.37
1	2	1323	A	N7-C5	-5.07	1.36	1.39
1	2	26	C	N3-C4	-5.04	1.30	1.33
1	2	1325	C	N1-C6	-5.02	1.34	1.37

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	7	2	ALA	C-N-CA	7.39	140.17	121.70
1	2	721	C	C2-N1-C1'	6.88	126.37	118.80
31	4	56	C	C2-N1-C1'	6.59	126.05	118.80
1	2	1388	C	C2-N1-C1'	6.34	125.78	118.80
1	2	437	U	N1-C2-O2	6.26	127.18	122.80
1	2	1114	G	C4-N9-C1'	6.22	134.59	126.50
1	2	494	C	N3-C2-O2	-6.16	117.59	121.90
1	2	321	G	N3-C4-N9	6.12	129.67	126.00
1	2	1114	G	C8-N9-C1'	-6.10	119.07	127.00
1	2	1033	G	N3-C4-C5	-6.07	125.56	128.60
1	2	437	U	N3-C2-O2	-6.04	117.97	122.20
1	2	618	C	C2-N1-C1'	6.00	125.40	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1114	G	N3-C4-N9	5.95	129.57	126.00
1	2	494	C	N1-C2-O2	5.94	122.47	118.90
1	2	962	G	N3-C4-N9	5.92	129.55	126.00
1	2	759	A	O4'-C1'-N9	5.86	112.88	108.20
1	2	119	C	C6-N1-C2	-5.81	117.97	120.30
1	2	302	C	C2-N1-C1'	5.75	125.12	118.80
33	7	93	ASP	C-N-CA	5.73	136.03	121.70
1	2	1132	C	C2-N1-C1'	5.63	124.99	118.80
1	2	321	G	N3-C4-C5	-5.53	125.83	128.60
1	2	396	C	N3-C4-N4	5.48	121.84	118.00
1	2	393	C	C2-N1-C1'	5.46	124.81	118.80
1	2	290	G	C4-N9-C1'	5.41	133.53	126.50
1	2	1400	C	C6-N1-C2	-5.40	118.14	120.30
1	2	1033	G	C4-N9-C1'	5.38	133.50	126.50
1	2	1189	C	C2-N1-C1'	5.38	124.72	118.80
1	2	1037	G	N3-C4-N9	5.37	129.22	126.00
1	2	576	U	N3-C2-O2	-5.32	118.48	122.20
1	2	396	C	C5-C4-N4	-5.31	116.48	120.20
1	2	1155	G	C4-N9-C1'	-5.30	119.61	126.50
1	2	693	C	C6-N1-C2	-5.27	118.19	120.30
1	2	536	C	C2-N1-C1'	5.26	124.59	118.80
1	2	641	G	C5-C6-O6	5.26	131.76	128.60
1	2	559	G	N3-C4-C5	-5.25	125.97	128.60
1	2	420	G	N3-C4-N9	5.22	129.13	126.00
1	2	443	G	C4-N9-C1'	5.21	133.27	126.50
1	2	962	G	C4-N9-C1'	5.19	133.25	126.50
1	2	1033	G	N3-C4-N9	5.15	129.09	126.00
1	2	1109	G	C4-N9-C1'	5.14	133.19	126.50
1	2	962	G	C8-N9-C1'	-5.12	120.35	127.00
1	2	551	C	C6-N1-C2	-5.07	118.27	120.30
1	2	105	A	N1-C6-N6	-5.07	115.56	118.60
1	2	981	C	N1-C2-O2	5.00	121.90	118.90
20	S	16	LEU	CA-CB-CG	5.00	126.80	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
35	9	167	GLU	Peptide
26	Y	8	TYR	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	32291	0	16317	236	0
2	A	1533	0	1627	32	0
3	B	1571	0	1630	23	0
4	C	482	0	462	11	0
5	D	1470	0	1542	15	0
6	E	1983	0	2060	33	0
7	F	1808	0	1879	29	0
8	G	977	0	1037	27	0
9	H	1720	0	1775	33	0
10	I	1034	0	1069	21	0
11	J	996	0	1076	17	0
12	K	1065	0	1121	18	0
13	L	817	0	871	16	0
14	M	964	0	994	15	0
15	N	1148	0	1248	22	0
16	O	1151	0	1191	23	0
17	P	455	0	475	7	0
18	Q	1262	0	1331	27	0
19	R	900	0	922	18	0
20	S	558	0	595	12	0
21	T	1057	0	1131	25	0
22	U	1223	0	1263	19	0
23	V	790	0	806	15	0
24	W	481	0	512	16	0
25	X	536	0	571	12	0
26	Y	408	0	413	13	0
27	Z	1550	0	1637	22	0
28	0	343	0	407	6	0
29	3	941	0	994	68	0
30	5	430	0	215	3	0
31	4	1622	0	830	64	0
32	6	777	0	806	42	0
33	7	3213	0	3331	196	0
34	8	1033	0	1074	45	0
35	9	2033	0	2145	118	0
36	2	30	0	0	0	0
36	4	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	5	2	0	0	0	0
36	7	1	0	0	0	0
37	C	2	0	0	0	0
37	F	1	0	0	0	0
37	P	1	0	0	0	0
37	R	1	0	0	0	0
37	W	1	0	0	0	0
38	4	8	0	8	4	0
39	7	32	0	13	1	0
40	2	39	0	0	7	0
40	K	1	0	0	0	0
40	Q	1	0	0	0	0
40	U	1	0	0	0	0
All	All	70744	0	55378	1185	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 9.

All (1185) 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)
33:7:241:SER:OG	33:7:294:LEU:HD23	1.32	1.24
33:7:51:TYR:CD1	33:7:294:LEU:HD12	1.79	1.17
21:T:124:ARG:HH21	21:T:124:ARG:HB3	1.13	1.14
19:R:16:CYS:SG	19:R:24:HIS:CE1	2.42	1.12
33:7:51:TYR:CE1	33:7:294:LEU:HG	1.87	1.10
33:7:51:TYR:HE1	33:7:294:LEU:HG	1.02	1.09
33:7:241:SER:HG	33:7:294:LEU:HD23	1.22	1.01
33:7:51:TYR:CE1	33:7:294:LEU:CG	2.46	0.99
31:4:76:A:H3'	38:4:101:MET:O	1.63	0.98
33:7:240:GLY:O	33:7:294:LEU:HA	1.64	0.96
33:7:51:TYR:HE1	33:7:294:LEU:CG	1.79	0.95
29:3:54:ALA:HA	29:3:80:VAL:HB	1.48	0.95
1:2:1020:A:N3	27:Z:135:LYS:NZ	2.16	0.94
1:2:1397:G:H1	1:2:1446:U:H3	1.18	0.91
1:2:835:A:H5'	7:F:151:SER:HB2	1.53	0.91
33:7:190:ASN:HD21	34:8:10:MET:HG3	1.36	0.90
33:7:51:TYR:HD1	33:7:294:LEU:HD12	1.32	0.90
19:R:16:CYS:SG	19:R:77:CYS:HB3	2.12	0.89
31:4:47:U:H5"	31:4:48:C:H5'	1.54	0.89
35:9:245:GLN:O	35:9:248:SER:HB3	1.73	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:7:9:GLU:O	33:7:207:ARG:NH1	2.07	0.87
33:7:51:TYR:CD1	33:7:294:LEU:CD1	2.56	0.87
1:2:1130:G:N7	20:S:44:LYS:NZ	2.24	0.86
1:2:1219:G:OP2	22:U:41:LYS:NZ	2.09	0.86
1:2:1309:C:O2'	9:H:175:ARG:NH1	2.09	0.86
33:7:240:GLY:O	33:7:294:LEU:CA	2.24	0.85
33:7:241:SER:OG	33:7:294:LEU:CD2	2.23	0.84
34:8:103:TYR:HB3	34:8:116:LEU:HD11	1.60	0.84
33:7:15:VAL:HG23	33:7:116:LEU:HD13	1.59	0.83
33:7:276:ILE:HA	33:7:299:THR:HG22	1.60	0.83
33:7:134:VAL:HG21	33:7:336:LEU:HD21	1.60	0.83
3:B:25:THR:HG22	3:B:27:ASP:H	1.43	0.82
31:4:52:G:H2'	31:4:53:G:C8	2.15	0.82
21:T:124:ARG:HH21	21:T:124:ARG:CB	1.92	0.81
1:2:877:G:N7	28:0:2:LYS:NZ	2.29	0.81
1:2:975:G:H2'	1:2:1000:G:H22	1.43	0.81
1:2:988:A:OP1	21:T:50:LYS:NZ	2.13	0.81
31:4:54:5MU:O2	31:4:58:A:N6	2.14	0.81
33:7:401:ILE:HD13	33:7:406:ARG:HB2	1.63	0.80
34:8:35:ILE:HB	34:8:89:SER:HA	1.63	0.80
2:A:90:ARG:O	2:A:94:ARG:HB2	1.81	0.80
35:9:222:ILE:HG23	35:9:226:ARG:HE	1.45	0.80
33:7:390:SER:H	33:7:393:ILE:HD11	1.45	0.80
3:B:151:ASP:OD1	4:C:42:ARG:NH1	2.16	0.79
31:4:62:C:H2'	31:4:63:G:H8	1.49	0.78
35:9:132:LYS:HD3	35:9:142:LYS:HE3	1.66	0.78
33:7:51:TYR:CE1	33:7:294:LEU:HB2	2.17	0.77
31:4:76:A:H3'	38:4:101:MET:C	2.04	0.77
35:9:9:PRO:HD2	35:9:78:VAL:HG11	1.66	0.77
1:2:1399:C:H2'	1:2:1400:C:H6	1.49	0.77
31:4:4:G:H2'	31:4:5:G:H8	1.50	0.77
10:I:42:GLN:NE2	10:I:48:GLY:O	2.17	0.76
35:9:151:LEU:HD13	35:9:161:VAL:HA	1.67	0.76
35:9:103:LEU:HD23	35:9:106:ILE:HD11	1.67	0.76
33:7:8:PRO:O	33:7:292:GLY:O	2.02	0.76
33:7:218:ILE:HD11	33:7:294:LEU:HD13	1.67	0.76
33:7:329:ILE:HG12	33:7:382:LEU:HD11	1.67	0.76
12:K:47:GLU:OE1	12:K:79:ARG:NH1	2.19	0.75
19:R:16:CYS:HG	19:R:24:HIS:CE1	2.04	0.75
29:3:15:LEU:HD11	29:3:117:LYS:HD2	1.68	0.75
2:A:97:VAL:O	2:A:98:ARG:NH1	2.18	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:7:170:THR:OG1	33:7:171:LYS:NZ	2.18	0.75
33:7:3:TRP:HZ2	33:7:83:PRO:HG2	1.51	0.75
35:9:70:ARG:HB2	35:9:79:ASP:HB2	1.69	0.75
34:8:51:CYS:HB3	34:8:56:ARG:HB3	1.68	0.75
1:2:1300:C:OP1	22:U:39:ARG:NH2	2.19	0.75
6:E:141:ASN:ND2	6:E:147:ASN:OD1	2.19	0.75
11:J:43:ARG:HH21	11:J:57:LEU:HD21	1.52	0.75
16:O:113:ARG:NH1	16:O:121:GLU:OE2	2.19	0.74
17:P:9:ARG:HG2	17:P:10:LYS:H	1.51	0.74
35:9:207:ILE:HD13	35:9:246:ILE:HD11	1.68	0.74
1:2:423:U:OP2	1:2:424:C:N4	2.20	0.74
29:3:3:LYS:HD3	29:3:4:PRO:HD2	1.70	0.74
33:7:246:LEU:HD11	33:7:248:LYS:HE3	1.70	0.74
1:2:264:G:OP1	19:R:98:LYS:NZ	2.21	0.73
6:E:87:ILE:HG22	6:E:88:MET:HG2	1.67	0.73
35:9:177:VAL:HG11	35:9:236:PRO:HB3	1.69	0.73
33:7:189:ILE:HG23	34:8:17:LYS:HB3	1.71	0.73
7:F:14:ASP:OD1	7:F:15:GLU:N	2.21	0.73
33:7:173:THR:HG23	33:7:175:ALA:H	1.51	0.73
34:8:137:LYS:HD3	34:8:138:PRO:HD2	1.70	0.73
35:9:247:ILE:HG21	35:9:263:VAL:HB	1.70	0.73
1:2:1292:A:O2'	21:T:69:ASP:OD2	2.06	0.72
31:4:52:G:H2'	31:4:53:G:H8	1.52	0.72
1:2:849:G:OP2	15:N:4:LYS:NZ	2.20	0.72
35:9:180:SER:OG	35:9:229:VAL:O	2.04	0.72
9:H:76:GLY:H	9:H:86:MET:HG3	1.54	0.72
9:H:215:ARG:NE	25:X:59:GLU:OE1	2.23	0.72
18:Q:38:VAL:HG21	18:Q:85:HIS:HD2	1.54	0.71
33:7:51:TYR:CE1	33:7:294:LEU:CB	2.72	0.71
6:E:188:THR:HG22	6:E:189:GLN:HG2	1.72	0.71
15:N:6:ALA:HB3	15:N:7:PRO:HD3	1.71	0.71
19:R:16:CYS:SG	19:R:77:CYS:CB	2.78	0.71
33:7:255:VAL:HA	33:7:316:ILE:HG12	1.72	0.71
33:7:207:ARG:NH2	33:7:291:PRO:HB2	2.04	0.71
33:7:209:LEU:HD22	33:7:246:LEU:HD23	1.72	0.71
1:2:991:G:OP1	17:P:2:ALA:N	2.23	0.71
8:G:37:GLN:OE1	8:G:60:LYS:NZ	2.23	0.71
33:7:213:PRO:HD2	33:7:318:LEU:HD11	1.73	0.71
19:R:16:CYS:SG	19:R:24:HIS:ND1	2.63	0.71
33:7:115:ILE:HD11	33:7:198:ILE:HG12	1.73	0.71
12:K:68:GLY:O	12:K:74:GLN:NE2	2.23	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:153:SER:OG	6:E:154:GLU:OE2	2.07	0.70
34:8:124:TYR:HB3	34:8:133:GLN:HG2	1.73	0.70
26:Y:17:ARG:HH22	29:3:44:GLU:HG3	1.57	0.70
35:9:214:LEU:HD12	35:9:233:GLY:HA3	1.74	0.70
32:6:68:ILE:HD11	32:6:84:TYR:HB3	1.73	0.70
24:W:39:CYS:HB3	24:W:43:GLY:H	1.57	0.70
26:Y:37:ARG:HA	26:Y:49:LYS:H	1.57	0.70
29:3:4:PRO:HD3	29:3:55:GLU:HB3	1.74	0.70
1:2:1115:G:HO2'	1:2:1116:A:H8	1.40	0.70
10:I:55:ASP:HB3	24:W:8:ILE:HG12	1.74	0.70
33:7:333:TYR:HA	33:7:410:TRP:O	1.91	0.70
31:4:76:A:O2'	33:7:280:ARG:HB3	1.91	0.69
35:9:68:VAL:HG22	35:9:80:VAL:HG12	1.74	0.69
33:7:48:LYS:NZ	33:7:309:ASP:OD2	2.24	0.69
1:2:725:G:N7	40:2:1708:HOH:O	2.25	0.69
35:9:178:LYS:HA	35:9:232:VAL:HG12	1.73	0.69
1:2:1193:4AC:O7	1:2:1193:4AC:H5	1.91	0.69
27:Z:83:GLN:HG3	27:Z:84:GLU:H	1.58	0.69
32:6:34:ALA:O	32:6:50:ARG:NH1	2.25	0.69
20:S:11:ARG:NH1	20:S:15:GLU:OE2	2.24	0.69
32:6:72:TRP:HB2	32:6:79:ARG:HD2	1.73	0.69
18:Q:104:ASN:OD1	18:Q:105:LEU:N	2.24	0.69
31:4:3:C:H2'	31:4:4:G:C8	2.27	0.69
31:4:62:C:H2'	31:4:63:G:C8	2.28	0.69
13:L:1:MET:HG2	13:L:2:GLN:H	1.58	0.69
35:9:199:VAL:HG11	35:9:261:ILE:HD12	1.75	0.69
32:6:47:ARG:HA	32:6:78:LYS:HA	1.73	0.69
35:9:250:LEU:HB3	35:9:261:ILE:HG21	1.74	0.69
10:I:106:THR:HG23	10:I:108:GLN:H	1.57	0.68
20:S:14:ARG:O	20:S:18:ASN:ND2	2.22	0.68
35:9:129:LEU:HD22	35:9:139:ALA:HB1	1.73	0.68
1:2:478:C:H2'	1:2:479:4AC:H6	1.75	0.68
27:Z:57:ARG:O	27:Z:60:ARG:NE	2.27	0.68
1:2:976:A:N7	1:2:1002:C:O2'	2.23	0.68
1:2:630:A:OP1	2:A:133:SER:OG	2.09	0.68
33:7:51:TYR:HD1	33:7:294:LEU:CD1	1.99	0.68
1:2:951:C:O2	17:P:12:ARG:NH1	2.27	0.68
33:7:182:PRO:HB2	34:8:14:LEU:HD22	1.76	0.68
27:Z:104:GLU:HA	27:Z:171:LEU:HD21	1.74	0.68
28:0:7:LYS:O	28:0:13:ARG:NH1	2.27	0.67
33:7:34:THR:HB	33:7:50:GLY:HA3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:44:ASP:OD1	3:B:45:VAL:N	2.27	0.67
1:2:825:U:O4	40:2:1701:HOH:O	2.08	0.67
25:X:18:THR:HG22	25:X:19:GLY:H	1.60	0.67
3:B:84:GLY:HA2	3:B:89:ALA:HB3	1.76	0.67
9:H:89:GLU:O	9:H:90:HIS:ND1	2.27	0.67
31:4:76:A:O3'	38:4:101:MET:HA	1.94	0.67
33:7:230:PHE:HA	33:7:233:LEU:HD21	1.77	0.66
1:2:1294:C:N4	21:T:69:ASP:OD1	2.28	0.66
33:7:167:LYS:O	33:7:170:THR:OG1	2.11	0.66
7:F:17:GLN:N	7:F:17:GLN:OE1	2.29	0.66
23:V:33:ARG:NH2	23:V:53:ILE:O	2.28	0.66
29:3:20:LEU:HD21	29:3:81:PRO:HD2	1.78	0.66
8:G:29:LEU:HA	8:G:32:LYS:HG2	1.77	0.66
13:L:30:THR:HG22	13:L:31:GLY:H	1.61	0.66
33:7:26:VAL:O	33:7:30:THR:OG1	2.13	0.66
33:7:255:VAL:HB	33:7:272:ILE:HB	1.76	0.66
33:7:56:ILE:HG13	33:7:86:LEU:HD13	1.78	0.66
33:7:242:ILE:HG13	33:7:295:VAL:HG11	1.76	0.66
1:2:1157:G:OP2	20:S:2:GLY:N	2.29	0.66
6:E:178:PRO:HD3	6:E:235:ARG:HH21	1.61	0.66
9:H:134:GLU:OE1	25:X:58:ARG:NH1	2.29	0.66
1:2:814:A:O2'	2:A:134:GLN:NE2	2.29	0.66
3:B:81:LYS:HE2	3:B:93:PRO:HG3	1.78	0.65
1:2:937:U:OP1	40:2:1702:HOH:O	2.14	0.65
29:3:92:ILE:HG13	29:3:93:GLU:H	1.60	0.65
8:G:40:VAL:O	8:G:44:GLY:N	2.28	0.65
29:3:101:ILE:HG13	29:3:104:PRO:HG3	1.78	0.65
2:A:145:ILE:HD11	2:A:171:ILE:HG12	1.78	0.65
34:8:55:ARG:HD3	34:8:115:ILE:HG21	1.78	0.65
31:4:76:A:H1'	33:7:237:VAL:HG21	1.78	0.65
23:V:43:MET:HG2	23:V:44:LEU:HD12	1.78	0.65
29:3:1:MET:HB3	29:3:53:ILE:HB	1.80	0.64
29:3:49:LYS:NZ	29:3:103:GLU:OE1	2.30	0.64
1:2:1446:U:H2'	1:2:1447:C:H6	1.62	0.64
11:J:103:THR:HG23	11:J:105:ILE:H	1.62	0.64
35:9:63:LYS:HD2	35:9:97:TRP:HZ2	1.62	0.64
1:2:280:C:OP1	11:J:87:ARG:NH1	2.31	0.64
1:2:972:G:O2'	1:2:1001:A:N1	2.26	0.64
15:N:36:ARG:O	15:N:40:LYS:NZ	2.31	0.64
21:T:124:ARG:HB3	21:T:124:ARG:NH2	1.99	0.64
29:3:107:ALA:HB1	29:3:110:LEU:HD21	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:8:127:CYS:HB3	34:8:131:GLY:H	1.62	0.64
23:V:25:HIS:O	23:V:25:HIS:ND1	2.31	0.64
34:8:125:ILE:H	34:8:133:GLN:HG3	1.62	0.64
1:2:948:G:OP1	40:2:1703:HOH:O	2.15	0.64
1:2:1446:U:H2'	1:2:1447:C:C6	2.33	0.64
11:J:86:ASN:OD1	11:J:87:ARG:N	2.31	0.64
1:2:782:A:OP1	28:0:3:ARG:NH2	2.31	0.63
21:T:83:VAL:HG12	21:T:84:HIS:H	1.62	0.63
33:7:136:LEU:HD13	33:7:144:LEU:HD21	1.80	0.63
2:A:152:GLU:OE1	2:A:152:GLU:N	2.26	0.63
18:Q:149:ASP:HB3	18:Q:151:GLU:HG2	1.79	0.63
31:4:8:4SU:O2'	31:4:21:A:N6	2.30	0.63
35:9:138:THR:O	35:9:142:LYS:HG2	1.98	0.63
1:2:923:G:OP2	16:O:130:ARG:NH1	2.32	0.63
15:N:39:GLU:O	15:N:40:LYS:HG2	1.99	0.63
18:Q:25:TRP:CD1	24:W:64:LEU:HD12	2.34	0.63
33:7:259:LEU:HD21	33:7:305:LEU:HG	1.80	0.63
1:2:446:U:OP2	23:V:89:ARG:NH2	2.32	0.63
1:2:1399:C:H2'	1:2:1400:C:C6	2.31	0.63
31:4:22:G:H2'	31:4:23:C:C6	2.34	0.63
35:9:219:ILE:HG23	35:9:229:VAL:HG12	1.79	0.63
1:2:323:G:N7	6:E:3:ARG:NH1	2.39	0.62
22:U:143:ILE:HG13	22:U:144:ILE:HD12	1.81	0.62
1:2:415:G:H21	5:D:123:GLN:HE22	1.47	0.62
34:8:31:PRO:HG2	34:8:50:TYR:HA	1.81	0.62
35:9:151:LEU:HB3	35:9:161:VAL:HG22	1.80	0.62
33:7:279:ILE:HG21	33:7:289:ALA:HB2	1.81	0.62
10:I:28:LYS:HB3	10:I:29:PRO:HD3	1.82	0.62
1:2:154:G:OP1	8:G:18:GLN:NE2	2.33	0.62
1:2:1105:G:N3	22:U:138:LYS:NZ	2.48	0.62
27:Z:88:PRO:O	27:Z:95:GLN:NE2	2.31	0.62
13:L:70:LYS:O	13:L:71:ARG:NH1	2.26	0.62
16:O:80:ASN:HB2	16:O:92:HIS:ND1	2.15	0.62
35:9:119:LYS:O	35:9:123:GLU:HG2	2.00	0.62
33:7:20:HIS:CD2	33:7:119:ALA:HB2	2.34	0.62
31:4:21:A:H2'	31:4:46:A:H61	1.64	0.61
1:2:1427:G:N2	8:G:77:ASP:OD1	2.26	0.61
31:4:3:C:H2'	31:4:4:G:H8	1.63	0.61
35:9:31:LEU:O	35:9:36:GLY:HA2	2.00	0.61
23:V:72:TYR:OH	23:V:82:GLU:OE2	2.07	0.61
33:7:241:SER:HG	33:7:294:LEU:CD2	2.07	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:9:176:LYS:HE2	35:9:215:LEU:HD23	1.81	0.61
8:G:49:GLU:HB2	8:G:50:LEU:HD12	1.81	0.61
3:B:13:LEU:HG	3:B:18:HIS:CE1	2.36	0.61
31:4:4:G:H2'	31:4:5:G:C8	2.35	0.61
33:7:51:TYR:CE1	33:7:294:LEU:CD1	2.83	0.61
1:2:89:G:H2'	1:2:90:G:C8	2.36	0.61
29:3:85:GLU:O	29:3:89:ALA:HB2	2.01	0.60
31:4:75:C:H4'	33:7:223:VAL:HG13	1.82	0.60
19:R:84:ASP:N	19:R:84:ASP:OD1	2.32	0.60
1:2:216:G:N1	1:2:226:U:O4	2.33	0.60
12:K:39:GLU:HG3	12:K:42:ARG:HH21	1.66	0.60
1:2:1212:A:OP2	40:2:1704:HOH:O	2.16	0.60
33:7:22:LYS:HZ1	33:7:94:ALA:HB3	1.66	0.60
1:2:1290:G:N2	1:2:1293:A:OP2	2.35	0.60
7:F:16:TRP:O	7:F:27:LYS:NZ	2.23	0.60
8:G:33:ARG:N	8:G:36:ASP:OD2	2.34	0.60
13:L:84:GLN:HA	13:L:87:ARG:NH1	2.16	0.60
3:B:121:ARG:NH2	3:B:144:GLU:OE2	2.35	0.60
6:E:103:LEU:HD13	6:E:243:PRO:HD3	1.83	0.60
32:6:51:ILE:HD12	32:6:52:PRO:HD2	1.82	0.60
33:7:17:HIS:CG	33:7:18:VAL:H	2.19	0.60
35:9:16:ILE:HG13	35:9:65:ILE:HG12	1.82	0.60
1:2:153:C:N4	1:2:154:G:N7	2.50	0.59
33:7:332:LYS:HD3	33:7:412:LEU:HD22	1.84	0.59
26:Y:40:CYS:SG	26:Y:44:GLY:N	2.75	0.59
33:7:28:ALA:HA	33:7:188:LYS:HE2	1.83	0.59
29:3:66:LEU:O	29:3:70:CYS:N	2.35	0.59
33:7:388:VAL:HG21	33:7:415:ILE:HG21	1.82	0.59
35:9:144:VAL:HG11	35:9:237:LYS:HG2	1.83	0.59
14:M:34:THR:HG23	14:M:36:ALA:H	1.67	0.59
1:2:1395:G:N2	1:2:1448:C:O2	2.35	0.59
13:L:56:GLU:N	13:L:56:GLU:OE1	2.35	0.59
33:7:271:PRO:HB2	33:7:273:PHE:CE1	2.38	0.59
10:I:66:LEU:HB3	10:I:68:LYS:HD3	1.85	0.59
26:Y:24:ARG:HH21	26:Y:45:TYR:HD1	1.49	0.59
31:4:21:A:H62	31:4:47:U:H4'	1.68	0.59
33:7:147:VAL:HG11	33:7:183:VAL:HG22	1.84	0.59
31:4:2:G:H2'	31:4:3:C:H4'	1.84	0.59
33:7:58:VAL:HG23	33:7:86:LEU:HD11	1.83	0.59
33:7:251:GLN:HE21	33:7:252:GLU:H	1.51	0.59
33:7:49:LEU:HD21	33:7:104:MET:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:7:194:LEU:O	33:7:198:ILE:HG13	2.01	0.59
35:9:197:LYS:O	35:9:201:SER:OG	2.19	0.59
1:2:748:A:OP2	1:2:767:G:N1	2.24	0.58
18:Q:106:ARG:NH2	18:Q:126:GLU:OE2	2.33	0.58
9:H:179:SER:OG	9:H:180:PHE:N	2.36	0.58
31:4:58:A:O2'	31:4:60:U:OP2	2.21	0.58
12:K:49:LEU:HD23	12:K:86:LEU:HD11	1.85	0.58
1:2:563:G:H21	10:I:124:ARG:HH21	1.52	0.58
9:H:20:ARG:HH12	9:H:105:LYS:HD2	1.69	0.58
24:W:10:MET:HE3	24:W:11:PRO:HD2	1.85	0.58
35:9:120:ASP:O	35:9:124:GLN:HG3	2.03	0.58
5:D:58:LEU:HD13	5:D:70:ARG:HA	1.85	0.58
25:X:66:GLU:OE2	25:X:67:ILE:N	2.32	0.58
29:3:53:ILE:HD11	29:3:79:TYR:CE1	2.39	0.58
8:G:98:GLU:HG3	8:G:99:LYS:H	1.67	0.58
18:Q:19:ARG:NH1	18:Q:23:PRO:HG3	2.18	0.58
19:R:84:ASP:HB3	19:R:108:ARG:O	2.02	0.58
10:I:104:VAL:HG22	10:I:125:LEU:HD23	1.85	0.58
29:3:50:LEU:HD13	29:3:104:PRO:HG2	1.85	0.58
35:9:103:LEU:HD21	35:9:137:ILE:N	2.19	0.58
2:A:12:ASP:O	2:A:15:LYS:N	2.35	0.57
22:U:19:ARG:NH1	22:U:135:GLU:OE1	2.36	0.57
31:4:74:C:H4'	31:4:75:C:H5'	1.87	0.57
7:F:151:SER:O	7:F:151:SER:OG	2.15	0.57
16:O:99:ASP:N	16:O:99:ASP:OD1	2.37	0.57
34:8:35:ILE:HG23	34:8:42:THR:HG23	1.85	0.57
31:4:76:A:O2'	33:7:296:ALA:HB3	2.04	0.57
35:9:114:LEU:HD11	35:9:163:PRO:HB2	1.87	0.57
27:Z:56:GLY:HA2	27:Z:61:ARG:HD3	1.86	0.57
1:2:779:G:O6	40:2:1705:HOH:O	2.16	0.57
16:O:57:GLU:OE1	16:O:57:GLU:N	2.31	0.57
33:7:166:ILE:O	33:7:170:THR:HG23	2.04	0.57
1:2:1398:G:HO2'	1:2:1399:C:H6	1.53	0.56
4:C:52:PRO:HA	4:C:63:PRO:HD3	1.86	0.56
9:H:170:SER:O	9:H:170:SER:OG	2.21	0.56
1:2:496:G:N2	32:6:54:LYS:HA	2.20	0.56
1:2:672:U:O4	14:M:41:ARG:NH1	2.38	0.56
4:C:5:VAL:HG12	4:C:7:LEU:H	1.71	0.56
33:7:26:VAL:HG11	33:7:34:THR:HG23	1.86	0.56
33:7:240:GLY:O	33:7:294:LEU:CB	2.53	0.56
1:2:89:G:H2'	1:2:90:G:H8	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1415:U:H2'	1:2:1416:C:C6	2.40	0.56
7:F:167:ILE:HG12	7:F:168:GLY:H	1.70	0.56
11:J:57:LEU:HG	11:J:118:GLY:HA2	1.88	0.56
29:3:17:GLU:OE1	29:3:21:GLN:NE2	2.38	0.56
7:F:139:HIS:ND1	7:F:182:ASP:OD2	2.39	0.56
18:Q:90:GLU:OE1	18:Q:90:GLU:N	2.39	0.55
23:V:6:THR:OG1	23:V:22:GLU:OE1	2.23	0.55
26:Y:27:PRO:O	29:3:45:ARG:NE	2.30	0.55
33:7:313:GLY:HA2	33:7:363:SER:HB2	1.89	0.55
34:8:98:ARG:HB2	34:8:98:ARG:NH1	2.21	0.55
6:E:168:VAL:HG23	6:E:169:PRO:HD3	1.87	0.55
15:N:96:PHE:O	15:N:144:LYS:NZ	2.39	0.55
18:Q:64:LYS:HG2	18:Q:77:THR:HG22	1.87	0.55
29:3:23:VAL:O	29:3:27:ARG:N	2.39	0.55
1:2:659:U:O2'	1:2:661:A:N7	2.29	0.55
9:H:47:THR:HG22	9:H:65:GLU:OE2	2.07	0.55
18:Q:27:GLU:N	18:Q:27:GLU:OE1	2.39	0.55
33:7:56:ILE:HG23	33:7:86:LEU:HB2	1.87	0.55
34:8:63:LYS:O	34:8:67:LYS:NZ	2.27	0.55
1:2:1415:U:H2'	1:2:1416:C:H6	1.72	0.55
9:H:135:ASP:OD2	25:X:46:ARG:NH1	2.35	0.55
27:Z:20:PHE:HE1	27:Z:23:LYS:HZ1	1.55	0.55
33:7:102:ALA:O	33:7:105:LEU:HB2	2.07	0.55
35:9:122:TRP:HA	35:9:125:VAL:HG12	1.89	0.55
35:9:162:LYS:HE3	35:9:212:GLU:HB2	1.88	0.55
35:9:222:ILE:HG12	35:9:226:ARG:HH21	1.72	0.55
35:9:231:VAL:HG22	35:9:243:LEU:HD13	1.89	0.55
2:A:40:ASP:OD1	2:A:40:ASP:N	2.35	0.55
31:4:8:4SU:HN3	31:4:13:C:N4	2.03	0.55
1:2:296:U:H4'	15:N:36:ARG:HH12	1.72	0.55
1:2:389:G:N2	1:2:392:A:OP2	2.23	0.55
1:2:1025:C:OP1	17:P:44:ARG:NH2	2.37	0.55
33:7:218:ILE:CD1	33:7:294:LEU:HD13	2.36	0.55
1:2:461:A:O2'	1:2:462:U:OP1	2.21	0.55
1:2:703:4AC:H5	1:2:703:4AC:O7	2.07	0.55
29:3:16:ALA:O	29:3:20:LEU:HB2	2.07	0.55
29:3:32:ILE:HD12	29:3:34:LYS:HD2	1.89	0.55
33:7:213:PRO:HB3	33:7:246:LEU:H	1.70	0.55
22:U:61:ARG:O	22:U:65:ASP:HB2	2.07	0.54
35:9:239:ALA:O	35:9:243:LEU:N	2.39	0.54
11:J:127:GLU:OE1	11:J:127:GLU:N	2.31	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Q:74:ARG:NH1	18:Q:80:ARG:HD3	2.23	0.54
24:W:20:CYS:SG	24:W:21:ILE:N	2.80	0.54
25:X:59:GLU:O	25:X:60:THR:OG1	2.19	0.54
34:8:55:ARG:HB3	34:8:115:ILE:HG12	1.90	0.54
12:K:10:ARG:NH1	12:K:110:ASP:OD2	2.40	0.54
1:2:1467:UR3:O5'	1:2:1467:UR3:H6	2.07	0.54
4:C:24:ARG:HH12	7:F:44:ILE:HD12	1.73	0.54
6:E:116:SER:OG	6:E:117:GLU:N	2.39	0.54
7:F:39:ARG:NH1	7:F:123:GLU:OE2	2.41	0.54
33:7:366:THR:HG21	33:7:382:LEU:HD23	1.90	0.54
6:E:80:ASP:OD1	6:E:83:PHE:HB2	2.08	0.54
9:H:16:LYS:O	9:H:43:LEU:HA	2.07	0.54
11:J:33:SER:HB3	11:J:56:ARG:HH11	1.73	0.54
34:8:98:ARG:HB2	34:8:98:ARG:HH11	1.73	0.54
35:9:54:ILE:HA	35:9:57:VAL:HG12	1.89	0.54
11:J:67:ASP:OD1	11:J:68:LYS:N	2.37	0.54
22:U:19:ARG:NH2	22:U:135:GLU:OE2	2.38	0.54
26:Y:38:TRP:N	26:Y:49:LYS:HB3	2.23	0.54
31:4:55:PSU:O2'	31:4:57:A:N7	2.36	0.54
34:8:68:GLU:HG3	34:8:98:ARG:HH12	1.73	0.54
6:E:9:HIS:O	6:E:31:ARG:NH1	2.41	0.54
32:6:24:LEU:HD13	32:6:71:PRO:HG3	1.90	0.54
34:8:42:THR:HB	34:8:83:ILE:HB	1.89	0.54
35:9:138:THR:HA	35:9:141:GLU:HB3	1.90	0.54
35:9:194:GLU:HA	35:9:197:LYS:HD2	1.88	0.54
16:O:21:LEU:HD22	16:O:40:CYS:SG	2.48	0.54
21:T:27:LEU:O	21:T:28:LEU:HD23	2.08	0.54
32:6:93:TRP:HE3	32:6:94:LEU:HD12	1.73	0.54
33:7:121:ASN:HD21	33:7:150:LYS:HD3	1.73	0.54
1:2:1183:C:H2'	1:2:1184:4AC:H5'	1.90	0.53
34:8:68:GLU:HB3	34:8:95:LEU:HD21	1.90	0.53
35:9:248:SER:HA	35:9:251:ILE:HD12	1.90	0.53
1:2:1239:4AC:O7	22:U:99:ARG:NH1	2.41	0.53
20:S:27:ASP:HB3	20:S:30:HIS:HB3	1.88	0.53
33:7:214:VAL:HB	33:7:244:GLN:HE21	1.72	0.53
2:A:113:LYS:HE2	2:A:152:GLU:HA	1.90	0.53
13:L:2:GLN:HB3	13:L:100:LEU:HD12	1.91	0.53
5:D:106:GLN:HE21	5:D:122:ARG:HB2	1.73	0.53
8:G:115:GLU:N	8:G:115:GLU:OE1	2.42	0.53
24:W:39:CYS:CB	24:W:42:CYS:SG	2.96	0.53
29:3:8:LYS:HE2	29:3:79:TYR:CE2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:6:20:GLU:O	32:6:23:GLN:HG3	2.08	0.53
1:2:81:U:H2'	1:2:82:C:C6	2.43	0.53
2:A:87:LYS:HG2	2:A:88:LEU:O	2.09	0.53
35:9:247:ILE:O	35:9:251:ILE:HG13	2.07	0.53
1:2:1095:A:H2'	1:2:1096:G:H8	1.74	0.53
33:7:240:GLY:O	33:7:294:LEU:HB3	2.09	0.53
1:2:204:G:O2'	11:J:64:ASN:OD1	2.23	0.53
31:4:6:G:H2'	31:4:7:G:O4'	2.08	0.53
31:4:46:A:H2'	31:4:47:U:H5'	1.89	0.53
29:3:2:ALA:O	29:3:55:GLU:HA	2.09	0.53
33:7:56:ILE:HD13	33:7:195:ILE:HG21	1.90	0.53
33:7:146:ILE:HG21	33:7:166:ILE:HG21	1.90	0.53
10:I:46:TYR:HD1	10:I:69:ILE:HG22	1.74	0.53
16:O:110:ARG:NH1	16:O:121:GLU:HG2	2.24	0.53
31:4:8:4SU:HN3	31:4:13:C:H41	1.57	0.53
1:2:29:C:O2'	1:2:884:A:N1	2.34	0.53
1:2:359:C:O2'	1:2:360:G:H5'	2.09	0.53
1:2:965:A:H2'	1:2:966:C:H5'	1.91	0.53
1:2:1383:C:H4'	32:6:32:LEU:HD13	1.91	0.53
1:2:1462:A:H2	32:6:51:ILE:HG21	1.73	0.53
31:4:68:C:H2'	31:4:69:C:O4'	2.09	0.52
33:7:16:GLY:H	33:7:132:HIS:CE1	2.26	0.52
35:9:246:ILE:HD13	35:9:249:ASN:HD22	1.73	0.52
1:2:224:G:O2'	1:2:225:C:O4'	2.28	0.52
35:9:16:ILE:HD13	35:9:97:TRP:HB2	1.90	0.52
1:2:641:G:OP1	2:A:119:ARG:NH1	2.42	0.52
12:K:63:ASP:OD1	12:K:63:ASP:N	2.41	0.52
33:7:213:PRO:HA	33:7:244:GLN:O	2.08	0.52
7:F:68:ILE:HG23	7:F:85:VAL:HG22	1.91	0.52
10:I:31:SER:OG	10:I:32:LYS:N	2.43	0.52
10:I:51:GLU:OE2	10:I:62:ARG:NH1	2.43	0.52
18:Q:67:ARG:HD2	18:Q:72:PRO:O	2.10	0.52
1:2:1462:A:C6	32:6:56:ARG:HA	2.45	0.52
8:G:81:PRO:HD3	8:G:111:THR:HB	1.91	0.52
9:H:137:THR:O	9:H:147:HIS:HA	2.09	0.52
33:7:330:ARG:HA	33:7:378:ILE:O	2.10	0.52
33:7:54:THR:O	33:7:89:ILE:N	2.37	0.52
33:7:132:HIS:O	33:7:136:LEU:HG	2.10	0.52
33:7:334:ASN:HB3	33:7:410:TRP:CE2	2.44	0.52
35:9:9:PRO:HB2	35:9:68:VAL:HG21	1.91	0.52
35:9:166:GLU:O	35:9:236:PRO:HD2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:861:G:O2'	1:2:877:G:O6	2.27	0.52
1:2:975:G:H2'	1:2:1000:G:N2	2.21	0.52
1:2:1236:C:H2'	1:2:1237:C:C6	2.45	0.52
14:M:89:SER:O	14:M:89:SER:OG	2.25	0.52
29:3:19:ALA:HB3	29:3:78:ILE:HD13	1.92	0.52
1:2:1115:G:O2'	1:2:1116:A:H8	1.92	0.52
1:2:1155:G:O2'	1:2:1156:G:O5'	2.27	0.52
31:4:50:U:H2'	31:4:51:C:C6	2.45	0.52
31:4:75:C:H3'	31:4:75:C:H6	1.74	0.52
33:7:124:PHE:CD1	33:7:125:PRO:HA	2.45	0.52
33:7:249:VAL:HG21	33:7:287:LYS:HD3	1.91	0.52
1:2:286:4AC:H5"	1:2:286:4AC:H6	1.92	0.52
1:2:636:4AC:HM73	1:2:703:4AC:HM73	1.92	0.52
33:7:134:VAL:HG11	33:7:340:VAL:HG21	1.92	0.52
33:7:252:GLU:OE1	33:7:275:LYS:HG3	2.09	0.52
35:9:95:LEU:O	35:9:99:LYS:HG2	2.10	0.52
1:2:1210:A:OP1	40:2:1706:HOH:O	2.19	0.51
6:E:205:PHE:HE2	6:E:212:VAL:HG23	1.76	0.51
10:I:76:LYS:HB3	10:I:77:PRO:HD3	1.91	0.51
1:2:683:C:O2'	14:M:124:ASP:OD2	2.13	0.51
1:2:1311:G:H5"	1:2:1312:G:OP1	2.10	0.51
4:C:49:LEU:HD12	4:C:49:LEU:O	2.11	0.51
9:H:44:LEU:HD12	9:H:45:PRO:HD2	1.93	0.51
14:M:31:THR:HG22	14:M:38:THR:HA	1.92	0.51
32:6:36:TRP:HZ3	32:6:48:ARG:HD3	1.75	0.51
33:7:110:LEU:HD22	33:7:241:SER:HB2	1.92	0.51
1:2:511:4AC:OP1	5:D:38:LYS:NZ	2.43	0.51
20:S:47:ARG:NH1	20:S:48:ASN:HD21	2.08	0.51
22:U:97:ILE:H	22:U:97:ILE:HD12	1.74	0.51
27:Z:67:ARG:HH21	27:Z:71:ARG:NH1	2.08	0.51
31:4:17:C:OP2	31:4:17(A):U:O2'	2.28	0.51
1:2:379:4AC:H5	1:2:379:4AC:O7	2.11	0.51
1:2:480:G:C6	1:2:481:G:N7	2.79	0.51
6:E:215:ILE:HD12	6:E:223:PHE:HE1	1.76	0.51
12:K:44:THR:O	12:K:79:ARG:HD3	2.10	0.51
32:6:16:VAL:HG21	32:6:94:LEU:HD11	1.91	0.51
35:9:1:MET:N	35:9:104:ASP:OD2	2.36	0.51
1:2:998:C:H2'	1:2:999:G:C8	2.45	0.51
1:2:1236:C:H2'	1:2:1237:C:H6	1.76	0.51
21:T:81:ILE:HD11	21:T:103:LEU:HD21	1.91	0.51
32:6:51:ILE:HG13	32:6:52:PRO:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:636:4AC:O7	1:2:636:4AC:H5	2.09	0.51
7:F:93:ASP:OD2	7:F:227:ARG:HA	2.10	0.51
1:2:973:A:N1	29:3:92:ILE:HG12	2.26	0.51
15:N:118:ASP:OD1	15:N:119:ILE:N	2.44	0.51
31:4:76:A:C2	33:7:278:SER:HB2	2.46	0.51
1:2:140:A:H5"	1:2:141:G:H5'	1.92	0.51
1:2:410:C:O2'	1:2:587:A:N3	2.41	0.51
1:2:1239:4AC:O7	1:2:1239:4AC:H5	2.11	0.51
23:V:5:ILE:HG22	23:V:21:PHE:HB3	1.92	0.51
30:5:823:C:H2'	30:5:824:A:C8	2.46	0.51
33:7:217:VAL:HG13	33:7:238:ILE:HG23	1.93	0.51
1:2:1260:U:OP2	22:U:72:ARG:NH1	2.38	0.51
13:L:45:ILE:HG12	13:L:66:LEU:HB3	1.91	0.51
33:7:120:ALA:HA	33:7:162:GLN:NE2	2.26	0.51
16:O:13:VAL:HG11	16:O:28:ILE:HA	1.92	0.50
35:9:193:VAL:HA	35:9:196:ILE:HG22	1.93	0.50
1:2:303:4AC:H5	1:2:303:4AC:O7	2.11	0.50
1:2:964:G:OP2	1:2:1186:A:N6	2.44	0.50
3:B:102:THR:O	7:F:45:LYS:NZ	2.44	0.50
15:N:37:LEU:HA	15:N:40:LYS:NZ	2.26	0.50
22:U:10:ASP:OD1	22:U:11:LEU:N	2.44	0.50
33:7:47:ILE:HA	33:7:100:LEU:HD13	1.94	0.50
1:2:1193:4AC:O5'	1:2:1193:4AC:H6	2.12	0.50
1:2:1397:G:N2	1:2:1446:U:O2	2.42	0.50
1:2:1414:A:H2'	1:2:1415:U:C6	2.47	0.50
18:Q:38:VAL:HG21	18:Q:85:HIS:CD2	2.42	0.50
32:6:87:THR:OG1	32:6:90:GLN:OE1	2.29	0.50
1:2:778:U:O2'	1:2:872:A:N1	2.44	0.50
1:2:1462:A:C2	32:6:51:ILE:HG12	2.46	0.50
20:S:14:ARG:NH2	20:S:53:TYR:OH	2.44	0.50
27:Z:147:TYR:O	27:Z:148:GLN:NE2	2.45	0.50
33:7:114:ALA:H	33:7:202:ILE:HD13	1.75	0.50
14:M:42:TRP:HH2	14:M:66:ARG:HH21	1.59	0.50
33:7:51:TYR:CE1	33:7:294:LEU:HD12	2.38	0.50
1:2:957:4AC:H5	1:2:957:4AC:O7	2.10	0.50
11:J:108:ALA:HB1	11:J:122:ALA:HB1	1.93	0.50
13:L:100:LEU:HD23	13:L:100:LEU:H	1.77	0.50
18:Q:19:ARG:HH11	18:Q:23:PRO:HG3	1.75	0.50
29:3:33:ARG:NH1	29:3:102:ILE:HD12	2.27	0.50
35:9:59:LYS:HD3	35:9:62:ARG:HE	1.76	0.50
35:9:224:ALA:HB3	35:9:225:PRO:HD3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Q:102:ALA:HB2	18:Q:125:ILE:HG21	1.94	0.50
33:7:351:ILE:HD11	33:7:408:ILE:HD12	1.93	0.50
1:2:223:G:H2'	1:2:224:G:C8	2.46	0.50
33:7:280:ARG:HH21	33:7:283:ASP:C	2.14	0.50
7:F:18:PRO:HG2	7:F:24:MET:SD	2.52	0.50
9:H:101:TYR:OH	12:K:39:GLU:OE1	2.29	0.50
29:3:23:VAL:HB	29:3:89:ALA:HB1	1.93	0.50
11:J:69:SER:O	11:J:69:SER:OG	2.30	0.49
31:4:10:G:H2'	31:4:11:A:O4'	2.11	0.49
34:8:54:ILE:HD12	34:8:104:VAL:HG21	1.94	0.49
1:2:1321:G:O6	12:K:10:ARG:NH2	2.43	0.49
24:W:47:VAL:HG22	24:W:56:ILE:HG22	1.93	0.49
29:3:31:LYS:O	29:3:101:ILE:HB	2.12	0.49
33:7:33:TRP:HD1	33:7:35:SER:HG	1.61	0.49
33:7:131:GLU:HG3	33:7:340:VAL:HG23	1.94	0.49
35:9:114:LEU:HD12	35:9:160:TRP:CZ3	2.47	0.49
2:A:71:VAL:HG12	2:A:81:THR:HG22	1.95	0.49
7:F:70:LEU:HD12	7:F:81:VAL:HG21	1.93	0.49
7:F:166:VAL:HG11	7:F:184:TRP:HD1	1.77	0.49
24:W:3:LEU:HD12	24:W:7:VAL:HG23	1.94	0.49
33:7:108:ALA:O	33:7:139:ILE:HG21	2.12	0.49
35:9:204:LEU:HD11	35:9:219:ILE:HG13	1.94	0.49
1:2:1032:A:N6	1:2:1074:A:H5'	2.27	0.49
29:3:52:ILE:HG22	29:3:78:ILE:HG12	1.93	0.49
29:3:70:CYS:SG	29:3:123:LYS:HG2	2.52	0.49
32:6:78:LYS:O	32:6:79:ARG:NH1	2.45	0.49
33:7:373:VAL:O	33:7:374:LYS:HD2	2.12	0.49
32:6:24:LEU:HD22	32:6:71:PRO:HB3	1.93	0.49
32:6:76:SER:O	32:6:76:SER:OG	2.29	0.49
35:9:220:TYR:O	35:9:228:ARG:N	2.38	0.49
13:L:84:GLN:HA	13:L:87:ARG:HH12	1.75	0.49
31:4:22:G:H2'	31:4:23:C:H6	1.78	0.49
16:O:3:ASP:OD1	16:O:3:ASP:N	2.45	0.49
23:V:51:THR:HG22	23:V:71:TYR:CD1	2.48	0.49
31:4:44:A:H2'	31:4:45:G:O4'	2.13	0.49
33:7:390:SER:OG	33:7:391:ASN:N	2.46	0.49
35:9:245:GLN:OE1	35:9:252:LYS:NZ	2.45	0.49
1:2:1155:G:O2'	1:2:1156:G:O4'	2.30	0.49
33:7:118:VAL:HG11	33:7:166:ILE:HD11	1.94	0.49
10:I:46:TYR:CD1	10:I:69:ILE:HG22	2.48	0.49
16:O:29:LYS:HB3	16:O:95:THR:HG22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Y:36:ASP:OD1	26:Y:48:TRP:NE1	2.46	0.49
35:9:125:VAL:HG13	35:9:126:ALA:N	2.28	0.49
5:D:55:ALA:HB2	5:D:73:LEU:HD21	1.95	0.49
33:7:311:LEU:H	33:7:311:LEU:HD23	1.78	0.49
35:9:185:VAL:HG13	35:9:261:ILE:HG12	1.95	0.49
1:2:1462:A:N1	32:6:51:ILE:HG12	2.28	0.48
1:2:1473:G:OP1	1:2:1476:A:H4'	2.13	0.48
21:T:79:LEU:HD23	21:T:79:LEU:H	1.78	0.48
26:Y:6:LYS:HG3	26:Y:7:LEU:HG	1.95	0.48
29:3:43:VAL:HG11	29:3:66:LEU:HD11	1.94	0.48
33:7:130:ARG:HB2	33:7:340:VAL:O	2.13	0.48
34:8:44:ILE:HG22	34:8:45:ARG:H	1.78	0.48
1:2:1414:A:H2'	1:2:1415:U:H6	1.79	0.48
3:B:32:ILE:HG21	3:B:41:TYR:HD2	1.79	0.48
20:S:27:ASP:OD1	20:S:28:PHE:N	2.47	0.48
24:W:36:ARG:HH12	24:W:48:GLU:HG2	1.77	0.48
29:3:42:ALA:HB1	29:3:47:GLN:HB2	1.95	0.48
35:9:185:VAL:HG22	35:9:261:ILE:HG12	1.94	0.48
1:2:83:C:H2'	1:2:84:C:C6	2.48	0.48
1:2:91:G:H2'	1:2:92:A:C8	2.48	0.48
2:A:53:LEU:HD13	2:A:67:LEU:HD11	1.94	0.48
25:X:70:ARG:O	25:X:71:ARG:HD3	2.14	0.48
33:7:3:TRP:CZ2	33:7:83:PRO:HG2	2.40	0.48
33:7:242:ILE:HG13	33:7:295:VAL:CG1	2.43	0.48
35:9:185:VAL:HB	35:9:227:TYR:CE2	2.48	0.48
1:2:278:C:H2'	1:2:279:A:H8	1.78	0.48
1:2:718:4AC:H5	1:2:718:4AC:O7	2.13	0.48
1:2:975:G:H8	1:2:975:G:OP2	1.96	0.48
6:E:106:ARG:NH2	6:E:195:ARG:HD2	2.29	0.48
24:W:39:CYS:SG	24:W:42:CYS:N	2.79	0.48
25:X:45:VAL:HG11	25:X:55:LEU:HD21	1.95	0.48
29:3:27:ARG:HD3	29:3:90:ALA:HA	1.95	0.48
33:7:57:GLY:HA2	33:7:84:LYS:O	2.14	0.48
1:2:75:G:H2'	1:2:76:G:C8	2.48	0.48
1:2:278:C:H2'	1:2:279:A:C8	2.47	0.48
14:M:131:GLY:O	14:M:133:ARG:N	2.46	0.48
33:7:160:LEU:O	33:7:164:ARG:HG2	2.12	0.48
35:9:100:ILE:HA	35:9:103:LEU:HD12	1.96	0.48
2:A:65:VAL:HG11	2:A:163:VAL:HG23	1.95	0.48
10:I:42:GLN:NE2	10:I:49:GLU:OE1	2.23	0.48
33:7:398:SER:HA	33:7:407:MET:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:8:101:LYS:HA	34:8:105:GLU:HG2	1.95	0.48
1:2:496:G:H22	32:6:54:LYS:HA	1.78	0.48
29:3:86:LEU:HB3	29:3:96:ALA:HB3	1.95	0.48
31:4:63:G:C2	31:4:64:G:C8	3.01	0.48
35:9:128:LYS:HB2	35:9:156:VAL:HG12	1.96	0.48
1:2:145:G:H2'	1:2:146:A:C8	2.49	0.48
29:3:67:PRO:HB2	29:3:68:PRO:HD3	1.96	0.48
33:7:327:TRP:NE1	33:7:382:LEU:O	2.46	0.48
33:7:359:LEU:HB2	33:7:366:THR:HG22	1.96	0.48
35:9:140:ILE:O	35:9:144:VAL:HG22	2.14	0.48
24:W:27:GLN:HE22	24:W:40:ASN:H	1.60	0.48
29:3:49:LYS:HG3	29:3:103:GLU:H	1.79	0.48
33:7:17:HIS:CE1	33:7:18:VAL:HG13	2.49	0.48
33:7:46:THR:HB	33:7:95:PRO:HA	1.94	0.48
33:7:192:ASP:OD1	34:8:13:ARG:NH2	2.47	0.48
35:9:183:ILE:HG13	35:9:227:TYR:HB2	1.96	0.48
35:9:215:LEU:HB2	35:9:233:GLY:HA2	1.95	0.48
1:2:286:4AC:OP1	19:R:71:HIS:NE2	2.46	0.48
1:2:626:4AC:H5	1:2:626:4AC:O7	2.13	0.48
6:E:69:GLY:HA2	6:E:77:VAL:HG21	1.96	0.48
6:E:138:ILE:HB	6:E:150:ILE:HG13	1.95	0.48
9:H:179:SER:HB3	9:H:182:GLU:HG2	1.96	0.48
13:L:18:GLU:HA	13:L:21:ASN:ND2	2.29	0.48
29:3:82:SER:OG	29:3:83:LYS:N	2.45	0.48
31:4:67:C:H2'	31:4:68:C:C6	2.49	0.48
33:7:29:ILE:HG21	33:7:91:PHE:CZ	2.49	0.48
33:7:332:LYS:O	33:7:411:GLY:HA2	2.13	0.48
1:2:1398:G:O2'	1:2:1399:C:H6	1.97	0.47
23:V:74:ASP:OD1	23:V:75:LYS:N	2.47	0.47
29:3:23:VAL:HA	29:3:26:ALA:HB3	1.97	0.47
29:3:50:LEU:HD21	29:3:111:VAL:HG22	1.96	0.47
29:3:72:GLU:OE1	29:3:72:GLU:N	2.47	0.47
34:8:5:LYS:HA	34:8:5:LYS:HD3	1.68	0.47
26:Y:6:LYS:HB3	29:3:62:ILE:HG12	1.94	0.47
32:6:55:LEU:C	32:6:57:ARG:H	2.17	0.47
33:7:359:LEU:HD22	33:7:397:ILE:HG13	1.96	0.47
1:2:306:G:N2	1:2:309:A:OP2	2.38	0.47
1:2:484:G:H5'	32:6:54:LYS:HE2	1.97	0.47
2:A:71:VAL:HA	2:A:81:THR:HA	1.96	0.47
9:H:99:LYS:O	9:H:103:VAL:HG13	2.14	0.47
1:2:520:G:OP1	15:N:38:LYS:NZ	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:10:ASP:OD1	8:G:12:LYS:N	2.47	0.47
8:G:30:ILE:HD11	8:G:114:PRO:HD3	1.95	0.47
9:H:131:ALA:HB2	9:H:161:ALA:HB2	1.95	0.47
10:I:50:PHE:HB3	10:I:63:VAL:HG22	1.95	0.47
16:O:16:ASP:OD1	16:O:17:GLY:N	2.38	0.47
29:3:74:GLU:O	29:3:123:LYS:NZ	2.47	0.47
33:7:151:VAL:HA	33:7:154:VAL:HG22	1.96	0.47
1:2:1206:C:O2'	12:K:130:ARG:NH2	2.43	0.47
9:H:185:ALA:O	9:H:189:ILE:HG12	2.14	0.47
27:Z:142:LYS:HG2	27:Z:143:SER:H	1.79	0.47
35:9:67:LYS:HE2	35:9:84:LYS:HG2	1.95	0.47
35:9:235:ASN:ND2	35:9:238:GLU:HB2	2.29	0.47
1:2:135:U:O2	6:E:147:ASN:ND2	2.45	0.47
1:2:914:G:OP1	9:H:89:GLU:HB3	2.14	0.47
8:G:17:LYS:HG3	8:G:50:LEU:HB3	1.97	0.47
33:7:94:ALA:HB1	33:7:104:MET:HB3	1.96	0.47
1:2:419:U:C2	1:2:420:G:C8	3.02	0.47
1:2:648:4AC:O7	1:2:648:4AC:H5	2.14	0.47
6:E:41:THR:HG22	6:E:189:GLN:HE22	1.79	0.47
9:H:88:ARG:O	9:H:88:ARG:HG3	2.15	0.47
10:I:90:GLU:HG3	10:I:94:LEU:HD12	1.96	0.47
19:R:30:HIS:O	19:R:30:HIS:ND1	2.43	0.47
29:3:26:ALA:HB1	29:3:104:PRO:HB3	1.96	0.47
29:3:32:ILE:HA	29:3:101:ILE:HG22	1.96	0.47
32:6:62:ARG:HG2	32:6:63:VAL:H	1.78	0.47
33:7:55:ASN:HA	33:7:88:ARG:HA	1.96	0.47
33:7:193:SER:HB2	34:8:13:ARG:HH21	1.79	0.47
33:7:240:GLY:O	33:7:295:VAL:N	2.48	0.47
35:9:14:ILE:HD11	35:9:65:ILE:HG22	1.97	0.47
35:9:135:ASP:O	35:9:138:THR:OG1	2.30	0.47
35:9:160:TRP:O	35:9:164:LEU:HB3	2.15	0.47
1:2:446:U:N3	1:2:449:A:OP2	2.36	0.47
1:2:1402:A:H2'	1:2:1403:G:H8	1.79	0.47
15:N:45:GLU:OE2	15:N:80:ASN:ND2	2.39	0.47
29:3:13:LYS:HD3	29:3:16:ALA:HB3	1.96	0.47
33:7:24:THR:C	33:7:185:ALA:HB1	2.35	0.47
34:8:119:GLU:HB3	34:8:122:SER:O	2.14	0.47
1:2:84:C:H2'	1:2:85:U:O4'	2.15	0.47
1:2:476:G:O2'	1:2:477:G:H5'	2.15	0.47
1:2:1157:G:O2'	1:2:1158:G:OP1	2.27	0.47
2:A:11:LYS:NZ	2:A:12:ASP:OD1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:5:VAL:HG13	4:C:8:LYS:HG2	1.96	0.47
3:B:27:ASP:HB3	3:B:147:LEU:HD12	1.97	0.47
11:J:120:VAL:O	11:J:121:ASN:ND2	2.48	0.47
21:T:50:LYS:HD2	21:T:59:TYR:CZ	2.49	0.47
21:T:65:THR:OG1	21:T:67:CYS:SG	2.60	0.47
33:7:241:SER:OG	33:7:294:LEU:HA	2.15	0.47
2:A:153:LEU:HD23	2:A:153:LEU:HA	1.71	0.46
2:A:196:GLU:OE1	2:A:196:GLU:N	2.42	0.46
12:K:92:ASP:OD1	12:K:95:LEU:HB3	2.15	0.46
15:N:63:LYS:HG2	15:N:118:ASP:O	2.16	0.46
33:7:233:LEU:HB2	35:9:197:LYS:HE2	1.97	0.46
35:9:114:LEU:HD12	35:9:160:TRP:HZ3	1.80	0.46
1:2:848:4AC:O3'	10:I:76:LYS:HG2	2.15	0.46
4:C:24:ARG:NH1	7:F:44:ILE:HD12	2.30	0.46
34:8:123:TRP:CD2	34:8:138:PRO:HB3	2.51	0.46
35:9:187:THR:OG1	35:9:259:VAL:HG13	2.16	0.46
1:2:153:C:C4	1:2:154:G:C8	3.02	0.46
1:2:1123:C:H2'	1:2:1124:U:C6	2.50	0.46
5:D:52:ARG:NH2	7:F:161:ARG:O	2.47	0.46
13:L:79:GLU:OE1	13:L:79:GLU:N	2.48	0.46
14:M:107:ARG:O	25:X:35:ARG:NH2	2.49	0.46
16:O:86:GLU:HG3	16:O:87:THR:HG22	1.98	0.46
26:Y:47:GLU:O	26:Y:50:LYS:NZ	2.48	0.46
27:Z:39:PRO:O	27:Z:40:LEU:HG	2.14	0.46
33:7:23:THR:O	33:7:26:VAL:HG12	2.14	0.46
33:7:146:ILE:O	33:7:180:ILE:HA	2.15	0.46
35:9:103:LEU:HA	35:9:106:ILE:HG12	1.96	0.46
1:2:223:G:H2'	1:2:224:G:H8	1.80	0.46
5:D:162:ASN:O	5:D:164:GLN:N	2.47	0.46
29:3:116:MET:HA	29:3:119:ARG:HB2	1.98	0.46
31:4:48:C:N4	31:4:59:A:H8	2.14	0.46
33:7:374:LYS:HB2	33:7:377:GLU:O	2.16	0.46
35:9:107:LEU:HD21	35:9:121:ALA:HB1	1.98	0.46
1:2:85:U:H2'	1:2:86:U:O4'	2.16	0.46
1:2:479:4AC:H5	1:2:479:4AC:O7	2.15	0.46
7:F:10:LYS:HD2	7:F:10:LYS:HA	1.79	0.46
8:G:32:LYS:HB3	8:G:36:ASP:OD2	2.15	0.46
27:Z:64:GLU:HA	27:Z:67:ARG:HG2	1.97	0.46
33:7:182:PRO:O	34:8:14:LEU:HD13	2.16	0.46
20:S:39:THR:OG1	20:S:41:VAL:HG23	2.16	0.46
1:2:1234:G:O2'	1:2:1235:A:H8	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:5:VAL:HA	4:C:8:LYS:HD3	1.98	0.46
13:L:43:LYS:NZ	27:Z:4:GLU:OE2	2.49	0.46
15:N:132:VAL:HG21	15:N:145:PRO:HD3	1.98	0.46
29:3:57:VAL:HG23	29:3:63:VAL:HG12	1.98	0.46
35:9:125:VAL:O	35:9:129:LEU:HB2	2.15	0.46
1:2:267:G:H5'	11:J:97:LYS:HB3	1.97	0.46
1:2:286:4AC:O7	1:2:286:4AC:H5	2.16	0.46
14:M:131:GLY:C	14:M:133:ARG:H	2.19	0.46
33:7:29:ILE:HG21	33:7:91:PHE:HZ	1.81	0.46
33:7:156:LYS:HG3	34:8:11:LEU:HD11	1.98	0.46
33:7:239:GLY:HA2	33:7:296:ALA:HA	1.98	0.46
1:2:1183:C:N4	1:2:1184:4AC:O7	2.48	0.46
1:2:1378:5HM:H11	1:2:1378:5HM:O5'	2.16	0.46
12:K:40:ILE:O	12:K:44:THR:OG1	2.34	0.46
17:P:16:LYS:NZ	17:P:28:GLY:O	2.47	0.46
18:Q:30:VAL:HG12	18:Q:66:PHE:HD2	1.81	0.46
31:4:56:C:H3'	31:4:57:A:H8	1.80	0.46
32:6:36:TRP:CZ3	32:6:48:ARG:HD3	2.51	0.46
1:2:798:U:O2'	1:2:1509:U:OP1	2.28	0.46
29:3:1:MET:HG3	29:3:63:VAL:O	2.15	0.46
32:6:55:LEU:O	32:6:59:VAL:HG22	2.16	0.46
32:6:66:LEU:O	32:6:86:TYR:HB2	2.16	0.46
33:7:260:ARG:NH1	33:7:262:GLU:HG2	2.31	0.46
33:7:356:THR:OG1	33:7:400:GLN:NE2	2.48	0.46
34:8:59:LYS:O	34:8:59:LYS:HD3	2.16	0.46
1:2:152:C:O2'	8:G:15:ILE:HG13	2.15	0.45
1:2:445:G:OP2	23:V:33:ARG:NH1	2.49	0.45
1:2:1420:U:O2'	1:2:1421:U:H2'	2.16	0.45
14:M:127:ARG:HG3	14:M:128:PRO:HD2	1.98	0.45
16:O:55:THR:HG23	16:O:58:GLN:HG3	1.98	0.45
25:X:18:THR:HB	25:X:24:VAL:HG23	1.98	0.45
33:7:300:TYR:HB3	35:9:191:LEU:HA	1.98	0.45
35:9:4:SER:OG	35:9:5:ARG:N	2.49	0.45
35:9:182:LEU:HD22	35:9:222:ILE:HG21	1.97	0.45
8:G:63:ILE:HG21	8:G:112:ILE:HD11	1.97	0.45
13:L:50:ARG:HG2	13:L:51:LYS:H	1.81	0.45
13:L:50:ARG:NH1	13:L:52:SER:OG	2.49	0.45
29:3:59:PRO:O	29:3:61:GLU:N	2.47	0.45
34:8:62:MET:O	34:8:66:LEU:HD23	2.16	0.45
35:9:165:LEU:HG	35:9:235:ASN:HD21	1.81	0.45
6:E:119:GLU:OE2	6:E:240:ILE:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:145:ARG:H	9:H:145:ARG:HD3	1.81	0.45
27:Z:109:PHE:CE2	27:Z:136:LEU:HD13	2.51	0.45
27:Z:128:VAL:HG23	27:Z:182:ILE:HG12	1.98	0.45
28:0:4:ARG:HH11	28:0:7:LYS:HE2	1.81	0.45
33:7:218:ILE:HG12	33:7:239:GLY:O	2.16	0.45
35:9:66:VAL:HG12	35:9:82:LEU:HB2	1.98	0.45
35:9:218:LYS:H	35:9:230:ASP:HB2	1.81	0.45
1:2:353:A:H5"	1:2:354:C:H5	1.82	0.45
1:2:636:4AC:CM7	1:2:703:4AC:HM73	2.46	0.45
13:L:30:THR:HG22	13:L:31:GLY:N	2.29	0.45
31:4:24:U:C2	31:4:25:C:C5	3.04	0.45
33:7:97:HIS:HB2	33:7:100:LEU:HD12	1.99	0.45
35:9:202:LYS:HG3	35:9:253:ILE:HG13	1.97	0.45
1:2:1379:G:H2'	1:2:1380:U:H6	1.80	0.45
2:A:15:LYS:HA	2:A:15:LYS:HD3	1.76	0.45
6:E:219:GLU:HG2	6:E:221:GLU:OE1	2.16	0.45
21:T:54:ALA:HA	21:T:58:LYS:O	2.17	0.45
22:U:129:LEU:HD23	22:U:129:LEU:HA	1.79	0.45
31:4:50:U:H2'	31:4:51:C:C5	2.51	0.45
33:7:150:LYS:HE2	39:7:501:GNP:C4	2.47	0.45
35:9:16:ILE:HG21	35:9:97:TRP:CE2	2.51	0.45
35:9:19:VAL:HG22	35:9:29:VAL:HG13	1.99	0.45
1:2:1290:G:O6	21:T:31:ARG:NH2	2.46	0.45
22:U:113:LYS:HE3	22:U:113:LYS:HB2	1.78	0.45
35:9:138:THR:HG22	35:9:141:GLU:OE2	2.17	0.45
1:2:1233:4AC:O7	1:2:1233:4AC:H5	2.16	0.45
5:D:78:LYS:HB3	5:D:78:LYS:HE2	1.61	0.45
28:0:32:LYS:O	28:0:34:ARG:N	2.50	0.45
29:3:13:LYS:O	29:3:17:GLU:HG2	2.17	0.45
33:7:12:ILE:HB	33:7:91:PHE:HD1	1.82	0.45
35:9:118:GLU:OE1	35:9:122:TRP:NE1	2.49	0.45
35:9:231:VAL:HG11	35:9:242:ALA:O	2.17	0.45
9:H:88:ARG:O	9:H:92:SER:HB3	2.15	0.45
15:N:137:LEU:HD21	15:N:144:LYS:HB2	1.99	0.45
33:7:43:ARG:NH2	33:7:47:ILE:HG22	2.32	0.45
35:9:10:SER:HB2	35:9:13:GLU:HB2	1.96	0.45
35:9:19:VAL:HA	35:9:29:VAL:HG13	1.99	0.45
1:2:1251:G:H2'	1:2:1253:A:H2	1.82	0.45
1:2:1378:5HM:OM5	1:2:1378:5HM:N4	2.47	0.45
10:I:76:LYS:HA	10:I:76:LYS:HD2	1.45	0.45
16:O:110:ARG:CZ	16:O:121:GLU:HG2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:3:36:THR:HG23	29:3:37:ASN:H	1.82	0.45
32:6:60:TRP:H	32:6:85:ARG:NH1	2.14	0.45
33:7:195:ILE:HA	33:7:198:ILE:HD12	1.97	0.45
1:2:1154:A:OP2	1:2:1154:A:H8	2.01	0.45
2:A:183:LYS:HA	2:A:183:LYS:HD3	1.70	0.45
3:B:57:LYS:NZ	4:C:34:ASN:OD1	2.24	0.45
4:C:53:TYR:HE1	4:C:63:PRO:HB3	1.81	0.45
7:F:105:GLU:OE2	27:Z:110:ARG:NE	2.50	0.45
9:H:197:LYS:HB3	9:H:197:LYS:HE3	1.78	0.45
31:4:10:G:N2	31:4:26:G:H1'	2.31	0.45
33:7:186:LEU:HD23	33:7:187:HIS:CD2	2.52	0.45
35:9:99:LYS:HB3	35:9:137:ILE:HG21	1.99	0.45
1:2:188:U:O2	1:2:189:A:N6	2.38	0.44
6:E:167:LYS:HG2	6:E:169:PRO:HD2	1.99	0.44
15:N:95:LYS:HE2	15:N:95:LYS:HB3	1.88	0.44
21:T:83:VAL:O	21:T:89:PHE:HA	2.17	0.44
22:U:141:GLU:OE1	22:U:148:LYS:HD3	2.17	0.44
33:7:230:PHE:CG	35:9:200:ILE:HG21	2.51	0.44
1:2:848:4AC:H5	1:2:848:4AC:O7	2.17	0.44
18:Q:100:LYS:HE3	18:Q:100:LYS:HB3	1.84	0.44
22:U:20:LEU:HD12	22:U:56:ALA:HB2	1.99	0.44
31:4:15:G:O2'	31:4:59:A:N6	2.51	0.44
31:4:19:G:N2	31:4:57:A:H1'	2.31	0.44
33:7:12:ILE:HB	33:7:91:PHE:CD1	2.52	0.44
33:7:17:HIS:CG	33:7:18:VAL:N	2.83	0.44
33:7:105:LEU:HD23	33:7:105:LEU:HA	1.66	0.44
35:9:107:LEU:HA	35:9:110:VAL:HG12	1.99	0.44
35:9:168:ALA:HB3	35:9:237:LYS:HD2	1.99	0.44
8:G:75:ARG:O	8:G:77:ASP:N	2.49	0.44
18:Q:109:LEU:HD11	18:Q:119:MET:HA	1.99	0.44
20:S:43:SER:OG	20:S:44:LYS:N	2.50	0.44
26:Y:10:VAL:HG23	26:Y:15:VAL:HG12	1.99	0.44
32:6:97:LYS:HB2	32:6:99:LYS:HG2	2.00	0.44
34:8:58:ASP:HB3	34:8:75:VAL:HG21	1.98	0.44
34:8:99:PHE:HA	34:8:103:TYR:CD2	2.53	0.44
3:B:97:LEU:HA	3:B:98:PRO:HD3	1.88	0.44
9:H:212:GLU:HG3	9:H:215:ARG:NH1	2.33	0.44
29:3:83:LYS:HA	29:3:86:LEU:HB2	1.99	0.44
30:5:822:C:H2'	30:5:823:C:C6	2.52	0.44
31:4:64:G:H2'	31:4:65:C:O4'	2.17	0.44
32:6:102:GLN:N	32:6:102:GLN:OE1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:7:220:SER:OG	33:7:306:THR:HB	2.18	0.44
1:2:1290:G:N1	1:2:1293:A:OP2	2.51	0.44
10:I:57:ARG:HH12	24:W:9:PRO:HD2	1.82	0.44
11:J:78:ILE:HB	11:J:102:GLU:OE2	2.17	0.44
31:4:49:G:H2'	31:4:50:U:C6	2.53	0.44
1:2:41:G:H4'	15:N:133:SER:OG	2.18	0.44
31:4:5:G:C2	31:4:6:G:C5	3.06	0.44
33:7:101:MET:O	33:7:104:MET:HG3	2.17	0.44
33:7:193:SER:HB2	34:8:13:ARG:NH2	2.32	0.44
34:8:118:LYS:HA	34:8:123:TRP:NE1	2.32	0.44
1:2:59:A:H4'	1:2:60:G:H5"	2.00	0.44
18:Q:68:ASP:OD1	18:Q:71:ASN:N	2.49	0.44
23:V:54:GLN:HB3	23:V:68:TYR:CD2	2.52	0.44
33:7:17:HIS:HB3	33:7:20:HIS:CE1	2.53	0.44
33:7:162:GLN:HG2	33:7:166:ILE:HD11	1.99	0.44
33:7:225:LYS:HG2	33:7:228:THR:OG1	2.16	0.44
35:9:14:ILE:HG23	35:9:93:LYS:HG2	1.99	0.44
8:G:9:SER:OG	8:G:121:VAL:O	2.33	0.44
8:G:87:LEU:HB2	8:G:104:LYS:NZ	2.33	0.44
16:O:60:LYS:HE3	16:O:60:LYS:HB3	1.82	0.44
16:O:103:ARG:O	16:O:107:MET:HG2	2.17	0.44
19:R:14:GLU:HG2	19:R:77:CYS:HB2	2.00	0.44
32:6:16:VAL:HG13	32:6:18:LEU:HG	2.00	0.44
33:7:59:CYS:SG	33:7:67:ALA:HB1	2.58	0.44
35:9:8:LEU:HB2	35:9:73:ARG:CZ	2.48	0.44
35:9:87:ASP:HA	35:9:90:ARG:HD3	1.99	0.44
35:9:218:LYS:O	35:9:230:ASP:N	2.50	0.44
3:B:36:ARG:HE	3:B:36:ARG:HB2	1.65	0.44
3:B:82:LYS:HA	3:B:82:LYS:HD3	1.75	0.44
7:F:166:VAL:HG11	7:F:184:TRP:CD1	2.53	0.44
15:N:37:LEU:HA	15:N:40:LYS:HZ3	1.83	0.44
17:P:13:LYS:HB2	17:P:13:LYS:HE3	1.81	0.44
33:7:11:ASN:HB3	33:7:111:MET:HA	2.00	0.44
1:2:144:G:N2	1:2:145:G:C4	2.86	0.43
2:A:12:ASP:OD1	2:A:13:LYS:N	2.51	0.43
2:A:20:TYR:HD1	2:A:77:GLN:HA	1.83	0.43
3:B:44:ASP:OD1	3:B:46:ARG:N	2.48	0.43
29:3:36:THR:HG23	29:3:37:ASN:N	2.33	0.43
29:3:52:ILE:O	29:3:52:ILE:HG13	2.17	0.43
32:6:69:VAL:HB	32:6:81:ASP:H	1.82	0.43
1:2:225:C:O2'	1:2:226:U:H5'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:4:18:G:O6	31:4:55:PSU:O2'	2.37	0.43
32:6:93:TRP:CH2	32:6:97:LYS:HD2	2.54	0.43
1:2:209:A:N3	1:2:231:C:O2'	2.50	0.43
1:2:1140:G:O6	1:2:1142:U:H5"	2.19	0.43
2:A:41:PRO:HB3	2:A:74:VAL:HG11	1.99	0.43
2:A:73:ASP:OD1	2:A:74:VAL:N	2.51	0.43
9:H:121:GLN:HA	9:H:124:VAL:HG12	1.99	0.43
18:Q:41:ARG:HD2	18:Q:41:ARG:HA	1.72	0.43
28:0:1:MET:SD	28:0:20:LYS:HE2	2.58	0.43
33:7:332:LYS:HB2	33:7:377:GLU:OE2	2.18	0.43
1:2:1260:U:OP2	22:U:72:ARG:HD3	2.19	0.43
3:B:169:TRP:HD1	3:B:195:PHE:CE2	2.35	0.43
12:K:34:GLU:N	12:K:34:GLU:OE1	2.52	0.43
21:T:93:GLU:OE2	21:T:95:LYS:NZ	2.45	0.43
33:7:22:LYS:NZ	33:7:94:ALA:HB3	2.32	0.43
33:7:254:LYS:HE2	33:7:318:LEU:O	2.17	0.43
34:8:88:SER:OG	34:8:89:SER:N	2.51	0.43
1:2:65:G:O6	1:2:365:A:N6	2.51	0.43
1:2:192:G:N2	1:2:195:A:OP2	2.46	0.43
1:2:997:C:O2'	26:Y:41:GLY:HA3	2.19	0.43
1:2:1356:C:H2'	1:2:1357:C:H6	1.83	0.43
16:O:81:ARG:NH2	16:O:105:ASP:OD2	2.48	0.43
19:R:43:PRO:HG2	19:R:46:THR:OG1	2.18	0.43
29:3:92:ILE:HG13	29:3:93:GLU:N	2.29	0.43
33:7:213:PRO:HB3	33:7:246:LEU:N	2.33	0.43
1:2:511:4AC:O7	1:2:511:4AC:H5	2.19	0.43
2:A:18:GLN:O	2:A:37:PRO:HA	2.18	0.43
6:E:219:GLU:H	6:E:219:GLU:CD	2.20	0.43
7:F:61:GLU:O	7:F:92:ARG:NH2	2.25	0.43
8:G:38:ILE:N	8:G:61:MET:O	2.51	0.43
18:Q:26:LEU:HA	18:Q:26:LEU:HD23	1.79	0.43
21:T:68:ARG:HB3	21:T:104:GLY:HA3	2.01	0.43
29:3:7:VAL:HG23	29:3:7:VAL:O	2.18	0.43
31:4:18:G:HO2'	31:4:19:G:C5'	2.31	0.43
33:7:274:THR:HB	33:7:301:LEU:HD21	1.99	0.43
1:2:205:G:H2'	1:2:206:C:C6	2.54	0.43
1:2:751:4AC:H5	1:2:751:4AC:O7	2.17	0.43
2:A:102:THR:HG21	2:A:130:ILE:HG12	1.99	0.43
10:I:55:ASP:OD1	10:I:55:ASP:N	2.50	0.43
33:7:184:SER:HB2	33:7:189:ILE:HD12	1.99	0.43
33:7:339:VAL:HG12	33:7:406:ARG:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:150:GLY:HA3	7:F:196:ASN:ND2	2.34	0.43
16:O:5:ARG:HG2	16:O:6:HIS:H	1.83	0.43
19:R:50:GLU:OE2	19:R:67:ARG:HD2	2.18	0.43
22:U:136:LEU:O	22:U:139:GLU:HG2	2.19	0.43
27:Z:121:MET:HG3	27:Z:148:GLN:HG3	2.01	0.43
34:8:47:PHE:HB3	34:8:80:GLU:HA	1.99	0.43
1:2:85:U:O2	1:2:89:G:N1	2.52	0.43
1:2:394:4AC:O7	1:2:394:4AC:H5	2.19	0.43
1:2:1296:C:OP1	21:T:110:ARG:NH2	2.52	0.43
9:H:25:ASP:OD1	9:H:25:ASP:N	2.51	0.43
18:Q:122:LEU:HD23	18:Q:122:LEU:HA	1.81	0.43
27:Z:38:THR:HG23	27:Z:39:PRO:O	2.19	0.43
33:7:192:ASP:OD1	33:7:193:SER:N	2.48	0.43
33:7:302:ASP:OD1	35:9:192:GLY:HA3	2.19	0.43
33:7:355:GLU:O	33:7:369:ILE:HA	2.18	0.43
35:9:4:SER:HB3	35:9:34:TYR:HD1	1.83	0.43
35:9:114:LEU:HD21	35:9:163:PRO:HB3	2.01	0.43
1:2:1432:G:H2'	1:2:1433:G:H8	1.82	0.43
3:B:47:LYS:HA	3:B:50:GLU:HG2	2.00	0.43
5:D:59:LEU:HD23	5:D:59:LEU:O	2.19	0.43
7:F:33:ASP:O	7:F:36:GLU:HG2	2.18	0.43
19:R:50:GLU:OE2	19:R:69:ARG:HD2	2.19	0.43
21:T:6:PHE:CE1	21:T:97:GLU:HG2	2.54	0.43
24:W:27:GLN:NE2	24:W:40:ASN:H	2.17	0.43
33:7:229:GLN:HE22	35:9:218:LYS:HB3	1.82	0.43
33:7:232:GLU:N	33:7:232:GLU:OE2	2.52	0.43
35:9:209:GLN:N	35:9:209:GLN:OE1	2.51	0.43
1:2:330:A:H2'	1:2:331:C:C6	2.54	0.42
1:2:1420:U:N3	1:2:1422:C:N3	2.66	0.42
8:G:76:PRO:HD2	8:G:92:PRO:HG3	2.00	0.42
16:O:45:LEU:HD12	16:O:49:MET:SD	2.59	0.42
23:V:32:SER:OG	23:V:33:ARG:N	2.52	0.42
23:V:51:THR:HG22	23:V:71:TYR:HD1	1.82	0.42
31:4:22:G:H2'	31:4:23:C:C5	2.54	0.42
32:6:28:VAL:HG12	32:6:39:VAL:HG12	2.01	0.42
1:2:17:4AC:H5	1:2:17:4AC:O7	2.19	0.42
1:2:97:A:H2'	1:2:98:C:H6	1.85	0.42
2:A:104:ILE:HG12	2:A:135:GLU:HG3	2.00	0.42
5:D:95:LEU:HD23	5:D:95:LEU:HA	1.91	0.42
5:D:168:ARG:NH1	5:D:172:GLU:OE2	2.52	0.42
9:H:135:ASP:OD1	9:H:136:THR:N	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:66:PHE:O	11:J:124:LEU:HB2	2.18	0.42
19:R:44:ARG:O	19:R:46:THR:HG23	2.18	0.42
21:T:121:GLY:HA2	21:T:127:MET:HG2	2.02	0.42
31:4:7:G:C4	31:4:49:G:C8	3.07	0.42
31:4:76:A:H3'	38:4:101:MET:CA	2.49	0.42
34:8:28:GLN:HE22	34:8:54:ILE:HG23	1.85	0.42
1:2:53:4AC:O7	1:2:53:4AC:H5	2.18	0.42
1:2:1041:4AC:H5	1:2:1041:4AC:O7	2.19	0.42
2:A:108:PHE:O	2:A:119:ARG:HA	2.19	0.42
6:E:233:VAL:HG23	6:E:233:VAL:O	2.19	0.42
25:X:59:GLU:OE2	25:X:59:GLU:N	2.53	0.42
29:3:24:GLU:HA	29:3:27:ARG:NH1	2.34	0.42
29:3:29:THR:HG21	29:3:105:GLY:O	2.19	0.42
31:4:14:A:H2'	31:4:14:A:N3	2.34	0.42
32:6:47:ARG:HB3	32:6:79:ARG:O	2.19	0.42
33:7:181:ILE:HG23	34:8:10:MET:HG2	2.00	0.42
3:B:183:SER:OG	3:B:187:GLU:OE1	2.31	0.42
10:I:18:GLU:HB3	10:I:65:LEU:HD13	2.02	0.42
31:4:70:G:H2'	31:4:71:C:C6	2.55	0.42
33:7:329:ILE:HD12	33:7:413:VAL:HG11	2.01	0.42
35:9:19:VAL:HA	35:9:29:VAL:HA	2.01	0.42
1:2:483:G:O2'	1:2:484:G:OP2	2.32	0.42
1:2:810:U:O2'	1:2:812:C:OP2	2.35	0.42
1:2:1267:G:OP1	9:H:3:LYS:HG3	2.19	0.42
8:G:111:THR:HG22	8:G:112:ILE:O	2.18	0.42
9:H:105:LYS:HB3	9:H:105:LYS:HE2	1.87	0.42
9:H:111:ILE:HG12	9:H:189:ILE:HD11	2.01	0.42
15:N:4:LYS:HB3	15:N:4:LYS:HE2	1.64	0.42
15:N:20:ARG:HD3	15:N:20:ARG:HA	1.76	0.42
32:6:88:GLN:HA	32:6:91:VAL:HG12	2.01	0.42
33:7:213:PRO:HA	33:7:245:GLY:HA3	2.01	0.42
34:8:56:ARG:HA	34:8:56:ARG:HE	1.84	0.42
1:2:263:G:OP1	19:R:97:THR:OG1	2.33	0.42
2:A:23:TYR:HD1	2:A:23:TYR:HA	1.69	0.42
6:E:196:LYS:HE2	6:E:196:LYS:HB2	1.92	0.42
8:G:118:GLN:NE2	8:G:120:ASN:OD1	2.46	0.42
12:K:101:LYS:HE2	12:K:101:LYS:HB3	1.83	0.42
15:N:31:LYS:HG2	15:N:35:LEU:HD12	2.01	0.42
15:N:54:VAL:HG12	15:N:101:ASP:H	1.84	0.42
16:O:125:PRO:HB3	16:O:129:GLN:OE1	2.19	0.42
29:3:74:GLU:HG2	29:3:76:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:7:162:GLN:HG2	33:7:166:ILE:CD1	2.50	0.42
33:7:229:GLN:NE2	35:9:218:LYS:HB3	2.35	0.42
35:9:198:GLU:HG2	35:9:257:GLU:OE2	2.19	0.42
1:2:641:G:H2'	1:2:642:U:C6	2.54	0.42
1:2:975:G:O6	29:3:38:GLU:HB2	2.19	0.42
7:F:70:LEU:H	7:F:70:LEU:HD23	1.85	0.42
7:F:210:LYS:HE3	7:F:210:LYS:HB3	1.60	0.42
11:J:41:ASP:OD1	11:J:41:ASP:N	2.53	0.42
18:Q:108:HIS:HD2	18:Q:109:LEU:HD23	1.85	0.42
19:R:16:CYS:HB2	19:R:24:HIS:CG	2.54	0.42
31:4:20:H2U:H3'	31:4:21:A:H4'	2.01	0.42
33:7:6:VAL:O	33:7:88:ARG:HD3	2.19	0.42
35:9:4:SER:HB3	35:9:34:TYR:CD1	2.54	0.42
1:2:973:A:N3	29:3:94:VAL:HG21	2.34	0.42
1:2:1025:C:O2'	13:L:52:SER:HB3	2.19	0.42
1:2:1095:A:H2'	1:2:1096:G:C8	2.54	0.42
5:D:103:ARG:HA	5:D:103:ARG:HD3	1.80	0.42
22:U:57:SER:O	22:U:61:ARG:HB2	2.20	0.42
31:4:59:A:H2'	31:4:60:U:H5'	2.01	0.42
33:7:26:VAL:HG23	33:7:91:PHE:CD2	2.55	0.42
35:9:102:ARG:O	35:9:105:LYS:HB3	2.19	0.42
1:2:680:G:H2'	1:2:681:G:C8	2.55	0.42
1:2:695:A:H2'	1:2:696:A:C8	2.55	0.42
1:2:975:G:O2'	1:2:1001:A:N6	2.53	0.42
1:2:977:A:C5	1:2:978:G:H1'	2.55	0.42
1:2:1277:C:H2'	1:2:1278:G:H5'	2.01	0.42
3:B:169:TRP:HD1	3:B:195:PHE:HE2	1.67	0.42
6:E:98:GLU:OE1	6:E:100:TYR:OH	2.36	0.42
8:G:47:LEU:HB3	8:G:49:GLU:HG2	2.01	0.42
1:2:569:G:OP1	6:E:191:LYS:NZ	2.52	0.42
1:2:1239:4AC:HM73	1:2:1240:G:O6	2.19	0.42
1:2:1397:G:H2'	1:2:1398:G:C8	2.55	0.42
3:B:121:ARG:HB2	3:B:145:ASN:HD21	1.84	0.42
5:D:106:GLN:NE2	5:D:122:ARG:HB2	2.35	0.42
7:F:185:SER:O	7:F:186:GLN:HG2	2.19	0.42
8:G:99:LYS:HD2	8:G:99:LYS:HA	1.69	0.42
9:H:20:ARG:HH12	9:H:105:LYS:CD	2.33	0.42
14:M:29:HIS:NE2	14:M:38:THR:OG1	2.40	0.42
19:R:39:VAL:HG22	19:R:48:THR:O	2.19	0.42
31:4:75:C:C3'	31:4:75:C:C6	3.03	0.42
2:A:11:LYS:HG2	2:A:12:ASP:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:32:LYS:HB3	20:S:32:LYS:HE2	1.82	0.41
27:Z:196:ILE:HD13	27:Z:196:ILE:HA	1.92	0.41
29:3:60:GLU:CD	29:3:63:VAL:HG21	2.40	0.41
31:4:23:C:N3	31:4:24:U:C5	2.88	0.41
33:7:230:PHE:HB2	35:9:200:ILE:HD13	2.00	0.41
35:9:105:LYS:O	35:9:109:LEU:HD23	2.19	0.41
35:9:152:ILE:HD11	35:9:161:VAL:HG11	2.02	0.41
1:2:839:4AC:O7	1:2:839:4AC:H5	2.19	0.41
14:M:135:ARG:O	14:M:137:VAL:N	2.51	0.41
18:Q:29:THR:HG22	18:Q:30:VAL:N	2.35	0.41
21:T:13:LEU:O	21:T:17:MET:N	2.53	0.41
33:7:249:VAL:HG23	33:7:287:LYS:O	2.20	0.41
33:7:330:ARG:O	33:7:413:VAL:HA	2.20	0.41
35:9:69:ILE:HB	35:9:70:ARG:HH11	1.85	0.41
1:2:1105:G:OP2	1:2:1106:C:N4	2.52	0.41
1:2:1151:G:H2'	1:2:1152:G:O4'	2.20	0.41
3:B:98:PRO:HB3	3:B:125:GLN:NE2	2.35	0.41
9:H:146:TYR:O	9:H:148:VAL:HG13	2.20	0.41
31:4:76:A:O2'	33:7:296:ALA:CB	2.68	0.41
35:9:20:LYS:HG2	35:9:30:SER:HB2	2.01	0.41
35:9:64:VAL:HG23	35:9:66:VAL:HG13	2.02	0.41
1:2:143:G:C2	1:2:144:G:C8	3.08	0.41
1:2:373:A2M:O5'	1:2:373:A2M:H8	2.20	0.41
1:2:974:U:OP2	29:3:36:THR:N	2.52	0.41
1:2:1379:G:H2'	1:2:1380:U:C6	2.55	0.41
6:E:217:ASP:OD1	6:E:217:ASP:N	2.52	0.41
7:F:148:LYS:HE2	7:F:148:LYS:HB3	1.87	0.41
12:K:38:PRO:HG2	12:K:41:ALA:HB3	2.01	0.41
33:7:15:VAL:HA	33:7:22:LYS:NZ	2.35	0.41
33:7:252:GLU:HG3	33:7:319:ALA:HB3	2.01	0.41
33:7:281:PHE:CE1	33:7:295:VAL:HB	2.54	0.41
6:E:178:PRO:HD3	6:E:235:ARG:NH2	2.30	0.41
6:E:191:LYS:HE2	6:E:191:LYS:HB3	1.72	0.41
23:V:70:LYS:HB2	23:V:70:LYS:HE3	1.79	0.41
30:5:823:C:H4'	32:6:57:ARG:HA	2.01	0.41
32:6:57:ARG:HG3	32:6:58:ARG:N	2.34	0.41
33:7:33:TRP:HD1	33:7:35:SER:OG	2.03	0.41
33:7:39:GLU:HG3	33:7:47:ILE:HD13	2.02	0.41
33:7:51:TYR:CZ	33:7:294:LEU:HB2	2.54	0.41
1:2:998:C:H2'	1:2:999:G:O4'	2.21	0.41
1:2:1023:G:H2'	1:2:1024:C:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:83:PHE:HA	6:E:84:PRO:HD3	1.91	0.41
8:G:10:ASP:OD1	8:G:13:THR:HG22	2.20	0.41
12:K:86:LEU:O	12:K:90:THR:HG22	2.21	0.41
18:Q:114:LYS:HB3	18:Q:114:LYS:HE2	1.80	0.41
20:S:57:LEU:HD23	20:S:57:LEU:HA	1.90	0.41
29:3:65:HIS:C	29:3:68:PRO:HD2	2.40	0.41
33:7:106:SER:HA	33:7:362:GLY:O	2.21	0.41
33:7:110:LEU:HD11	33:7:218:ILE:HG21	2.03	0.41
33:7:189:ILE:CG2	34:8:14:LEU:HD12	2.51	0.41
35:9:177:VAL:HG21	35:9:236:PRO:HD3	2.03	0.41
1:2:89:G:O2'	1:2:90:G:H5'	2.20	0.41
1:2:1354:U:O2'	1:2:1355:C:H5'	2.21	0.41
10:I:6:PRO:O	10:I:34:ILE:HD11	2.21	0.41
12:K:21:GLU:HG2	12:K:89:TRP:HZ2	1.86	0.41
31:4:17:C:H5"	31:4:17(A):U:H3'	2.02	0.41
31:4:22:G:H8	31:4:22:G:OP2	2.04	0.41
32:6:25:PHE:CD1	32:6:66:LEU:HD21	2.55	0.41
33:7:84:LYS:O	33:7:84:LYS:HG3	2.21	0.41
35:9:165:LEU:HG	35:9:235:ASN:ND2	2.36	0.41
1:2:868:4AC:O7	1:2:868:4AC:H5	2.20	0.41
1:2:1390:C:H2'	1:2:1391:G:O4'	2.20	0.41
4:C:29:HIS:HA	4:C:40:ILE:O	2.21	0.41
6:E:86:GLY:O	6:E:89:ASP:HB2	2.21	0.41
21:T:41:THR:O	21:T:45:LYS:HG3	2.20	0.41
24:W:56:ILE:CD1	24:W:60:ILE:HD11	2.50	0.41
29:3:113:GLU:HB2	29:3:114:ILE:HD12	2.01	0.41
34:8:115:ILE:HG22	34:8:116:LEU:N	2.36	0.41
1:2:43:U:O2'	1:2:465:G:O2'	2.21	0.41
1:2:97:A:H2'	1:2:98:C:C6	2.55	0.41
1:2:423:U:H5"	1:2:424:C:N3	2.36	0.41
1:2:1147:4AC:O7	1:2:1147:4AC:H5	2.21	0.41
1:2:1393:G:OP2	1:2:1393:G:H8	2.04	0.41
7:F:38:PHE:HZ	7:F:121:ILE:HG23	1.86	0.41
8:G:34:ILE:HD12	8:G:76:PRO:HB3	2.02	0.41
9:H:93:LEU:HD12	9:H:93:LEU:O	2.21	0.41
15:N:110:GLY:HA3	15:N:115:SER:O	2.20	0.41
29:3:32:ILE:C	29:3:33:ARG:HD2	2.41	0.41
29:3:34:LYS:HZ1	29:3:92:ILE:H	1.67	0.41
31:4:5:G:H2'	31:4:6:G:C8	2.56	0.41
33:7:62:CYS:SG	33:7:79:SER:OG	2.62	0.41
33:7:103:THR:O	33:7:106:SER:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:7:128:GLN:HA	33:7:341:GLY:HA2	2.02	0.41
35:9:203:ALA:HB1	35:9:250:LEU:HD22	2.03	0.41
1:2:1028:4AC:O7	1:2:1028:4AC:H5	2.21	0.41
18:Q:90:GLU:H	18:Q:90:GLU:CD	2.24	0.41
24:W:18:VAL:HG22	24:W:58:ALA:HB3	2.01	0.41
24:W:19:LYS:HE2	24:W:24:GLY:HA2	2.03	0.41
29:3:31:LYS:HE2	29:3:31:LYS:HB2	1.91	0.41
16:O:9:ARG:HE	16:O:9:ARG:HB2	1.62	0.40
18:Q:74:ARG:HH11	18:Q:80:ARG:HD3	1.84	0.40
21:T:84:HIS:CD2	21:T:86:GLY:H	2.39	0.40
27:Z:23:LYS:HE3	27:Z:23:LYS:HB3	1.90	0.40
34:8:49:GLU:HB3	34:8:53:ARG:CZ	2.51	0.40
34:8:68:GLU:HG3	34:8:98:ARG:NH1	2.36	0.40
1:2:64:U:H2'	1:2:65:G:C8	2.56	0.40
1:2:1093:C:O2'	1:2:1094:C:H5'	2.22	0.40
1:2:1296:C:O2'	1:2:1297:G:OP2	2.36	0.40
1:2:1487:MA6:H93	1:2:1488:MA6:H92	2.03	0.40
2:A:22:ILE:HB	2:A:33:VAL:O	2.21	0.40
5:D:88:VAL:HG12	5:D:89:LEU:H	1.87	0.40
16:O:5:ARG:HH11	16:O:8:VAL:HG22	1.85	0.40
23:V:7:GLU:HB3	23:V:20:TYR:HB2	2.02	0.40
25:X:18:THR:HG22	25:X:19:GLY:N	2.32	0.40
26:Y:38:TRP:HB2	26:Y:47:GLU:CD	2.41	0.40
27:Z:55:ILE:HA	27:Z:62:ILE:HD11	2.02	0.40
29:3:19:ALA:CB	29:3:78:ILE:HD13	2.51	0.40
33:7:340:VAL:H	33:7:340:VAL:HG22	1.60	0.40
1:2:982:A:N6	1:2:990:G:O6	2.55	0.40
1:2:1395:G:C2	1:2:1396:G:C8	3.10	0.40
1:2:1462:A:N6	32:6:56:ARG:HA	2.36	0.40
3:B:32:ILE:HG22	3:B:33:TYR:H	1.86	0.40
6:E:33:ARG:HG2	6:E:33:ARG:HH11	1.86	0.40
15:N:63:LYS:HA	15:N:63:LYS:HD2	1.72	0.40
18:Q:24:ILE:HD12	18:Q:24:ILE:H	1.86	0.40
21:T:76:MET:HA	21:T:79:LEU:HD21	2.03	0.40
32:6:39:VAL:HG23	32:6:47:ARG:HB2	2.02	0.40
33:7:361:VAL:HG22	33:7:395:THR:HG23	2.03	0.40
35:9:151:LEU:HD22	35:9:156:VAL:HG21	2.04	0.40
35:9:245:GLN:O	35:9:248:SER:CB	2.59	0.40
1:2:703:4AC:O5'	1:2:703:4AC:H6	2.22	0.40
1:2:1412:C:C2	1:2:1413:G:C8	3.10	0.40
5:D:131:GLU:OE1	5:D:155:ALA:HA	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:49:VAL:HG22	6:E:71:PHE:CZ	2.56	0.40
7:F:130:SER:OG	7:F:131:TRP:N	2.55	0.40
11:J:36:ARG:HA	11:J:93:ASN:O	2.22	0.40
12:K:130:ARG:HG2	12:K:131:GLN:H	1.87	0.40
14:M:32:ASP:OD2	14:M:34:THR:HG22	2.21	0.40
14:M:43:SER:HB2	14:M:46:MET:SD	2.62	0.40
17:P:34:HIS:CD2	27:Z:4:GLU:HG3	2.57	0.40
1:2:459:G:OP2	1:2:459:G:H8	2.05	0.40
1:2:651:G:H4'	14:M:37:GLU:OE1	2.22	0.40
1:2:996:G:O2'	1:2:997:C:P	2.80	0.40
2:A:32:GLU:H	2:A:32:GLU:CD	2.24	0.40
3:B:43:LEU:HD23	3:B:155:PRO:HB2	2.03	0.40
16:O:41:ARG:HD3	22:U:33:PRO:HB3	2.04	0.40
21:T:73:LEU:HD23	21:T:73:LEU:HA	1.87	0.40
33:7:36:LYS:HA	33:7:36:LYS:HD3	1.91	0.40
35:9:41:LEU:HD11	35:9:46:VAL:HG22	2.04	0.40
35:9:135:ASP:O	35:9:138:THR:N	2.48	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	
2	A	186/199 (94%)	158 (85%)	28 (15%)	0	100	100
3	B	194/202 (96%)	175 (90%)	19 (10%)	0	100	100
4	C	59/63 (94%)	51 (86%)	8 (14%)	0	100	100
5	D	173/180 (96%)	158 (91%)	15 (9%)	0	100	100
6	E	240/243 (99%)	206 (86%)	34 (14%)	0	100	100
7	F	227/236 (96%)	197 (87%)	30 (13%)	0	100	100
8	G	122/125 (98%)	95 (78%)	27 (22%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	H	211/215 (98%)	182 (86%)	29 (14%)	0	100	100
10	I	127/130 (98%)	114 (90%)	13 (10%)	0	100	100
11	J	124/127 (98%)	107 (86%)	17 (14%)	0	100	100
12	K	132/135 (98%)	116 (88%)	16 (12%)	0	100	100
13	L	99/102 (97%)	87 (88%)	12 (12%)	0	100	100
14	M	126/137 (92%)	109 (86%)	17 (14%)	0	100	100
15	N	144/147 (98%)	120 (83%)	24 (17%)	0	100	100
16	O	141/148 (95%)	125 (89%)	16 (11%)	0	100	100
17	P	53/56 (95%)	46 (87%)	7 (13%)	0	100	100
18	Q	150/158 (95%)	134 (89%)	16 (11%)	0	100	100
19	R	107/113 (95%)	91 (85%)	16 (15%)	0	100	100
20	S	64/67 (96%)	57 (89%)	7 (11%)	0	100	100
21	T	128/132 (97%)	109 (85%)	19 (15%)	0	100	100
22	U	147/150 (98%)	133 (90%)	14 (10%)	0	100	100
23	V	92/99 (93%)	82 (89%)	10 (11%)	0	100	100
24	W	61/65 (94%)	52 (85%)	9 (15%)	0	100	100
25	X	65/71 (92%)	45 (69%)	20 (31%)	0	100	100
26	Y	48/51 (94%)	30 (62%)	18 (38%)	0	100	100
27	Z	195/210 (93%)	163 (84%)	32 (16%)	0	100	100
28	0	34/36 (94%)	29 (85%)	5 (15%)	0	100	100
29	3	121/123 (98%)	93 (77%)	27 (22%)	1 (1%)	16	46
32	6	93/113 (82%)	77 (83%)	16 (17%)	0	100	100
33	7	412/415 (99%)	377 (92%)	35 (8%)	0	100	100
34	8	125/139 (90%)	114 (91%)	11 (9%)	0	100	100
35	9	248/266 (93%)	218 (88%)	30 (12%)	0	100	100
All	All	4448/4653 (96%)	3850 (87%)	597 (13%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
29	3	4	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	A	161/167 (96%)	161 (100%)	0	100 100
3	B	168/173 (97%)	168 (100%)	0	100 100
4	C	54/55 (98%)	54 (100%)	0	100 100
5	D	158/160 (99%)	157 (99%)	1 (1%)	84 90
6	E	213/214 (100%)	213 (100%)	0	100 100
7	F	192/198 (97%)	192 (100%)	0	100 100
8	G	107/108 (99%)	107 (100%)	0	100 100
9	H	183/184 (100%)	181 (99%)	2 (1%)	70 82
10	I	106/107 (99%)	106 (100%)	0	100 100
11	J	102/103 (99%)	102 (100%)	0	100 100
12	K	110/111 (99%)	109 (99%)	1 (1%)	75 85
13	L	90/91 (99%)	90 (100%)	0	100 100
14	M	95/104 (91%)	95 (100%)	0	100 100
15	N	120/121 (99%)	118 (98%)	2 (2%)	56 74
16	O	119/123 (97%)	119 (100%)	0	100 100
17	P	45/46 (98%)	45 (100%)	0	100 100
18	Q	137/143 (96%)	135 (98%)	2 (2%)	60 77
19	R	98/102 (96%)	96 (98%)	2 (2%)	50 71
20	S	60/61 (98%)	60 (100%)	0	100 100
21	T	113/114 (99%)	112 (99%)	1 (1%)	75 85
22	U	126/127 (99%)	126 (100%)	0	100 100
23	V	86/90 (96%)	86 (100%)	0	100 100
24	W	54/56 (96%)	54 (100%)	0	100 100
25	X	57/60 (95%)	56 (98%)	1 (2%)	54 74
26	Y	41/42 (98%)	38 (93%)	3 (7%)	11 35
27	Z	156/168 (93%)	156 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
28	0	34/34 (100%)	34 (100%)	0	100 100
29	3	99/99 (100%)	99 (100%)	0	100 100
32	6	83/99 (84%)	83 (100%)	0	100 100
33	7	356/357 (100%)	356 (100%)	0	100 100
34	8	118/126 (94%)	118 (100%)	0	100 100
35	9	227/239 (95%)	226 (100%)	1 (0%)	89 93
All	All	3868/3982 (97%)	3852 (100%)	16 (0%)	88 93

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	D	168	ARG
9	H	133	ARG
9	H	145	ARG
12	K	16	ARG
15	N	32	ARG
15	N	131	ARG
18	Q	84	LYS
18	Q	130	ARG
19	R	8	ARG
19	R	69	ARG
21	T	124	ARG
25	X	71	ARG
26	Y	17	ARG
26	Y	37	ARG
26	Y	40	CYS
35	9	83	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	77	GLN
2	A	134	GLN
3	B	18	HIS
3	B	145	ASN
3	B	178	ASN
5	D	106	GLN
5	D	123	GLN
5	D	135	GLN

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Mol	Chain	Res	Type
5	D	164	GLN
6	E	99	HIS
7	F	181	GLN
7	F	203	ASN
8	G	118	GLN
8	G	120	ASN
9	H	193	ASN
10	I	9	ASN
11	J	121	ASN
15	N	130	ASN
16	O	72	HIS
18	Q	85	HIS
19	R	99	HIS
20	S	48	ASN
21	T	84	HIS
24	W	27	GLN
24	W	40	ASN
25	X	26	GLN
27	Z	72	GLN
27	Z	79	GLN
27	Z	95	GLN
27	Z	148	GLN
33	7	11	ASN
33	7	132	HIS
33	7	148	GLN
33	7	187	HIS
33	7	190	ASN
33	7	244	GLN
33	7	251	GLN
33	7	400	GLN
34	8	28	GLN
35	9	249	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1458/1497 (97%)	322 (22%)	6 (0%)
30	5	19/20 (95%)	7 (36%)	0
31	4	75/76 (98%)	33 (44%)	1 (1%)
All	All	1552/1593 (97%)	362 (23%)	7 (0%)

All (362) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	14	U
1	2	16	C
1	2	23	A
1	2	29	C
1	2	40	U
1	2	45	U
1	2	52	C
1	2	55	A
1	2	57	U
1	2	59	A
1	2	62	C
1	2	72	A
1	2	73	A
1	2	74	G
1	2	82	C
1	2	86	U
1	2	88	U
1	2	89	G
1	2	90	G
1	2	91	G
1	2	99	C
1	2	104	G
1	2	112	A
1	2	113	G
1	2	117	C
1	2	126	A
1	2	128	C
1	2	140	A
1	2	146	A
1	2	154	G
1	2	157	A
1	2	160	C
1	2	170	U
1	2	174	C
1	2	196	G
1	2	197	G
1	2	209	A
1	2	210	A
1	2	211	A
1	2	212	G
1	2	217	C
1	2	221	A
1	2	222	A

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Mol	Chain	Res	Type
1	2	223	G
1	2	225	C
1	2	226	U
1	2	227	C
1	2	229	G
1	2	236	G
1	2	240	G
1	2	249	C
1	2	251	G
1	2	254	U
1	2	256	G
1	2	260	G
1	2	262	U
1	2	275	G
1	2	276	C
1	2	277	C
1	2	288	A
1	2	292	U
1	2	294	G
1	2	298	C
1	2	308	G
1	2	315	A
1	2	337	C
1	2	338	A
1	2	341	G
1	2	353	A
1	2	354	C
1	2	355	G
1	2	358	G
1	2	361	C
1	2	362	A
1	2	363	G
1	2	373	A2M
1	2	374	A
1	2	375	C
1	2	376	C
1	2	381	C
1	2	384	U
1	2	397	G
1	2	402	G
1	2	406	A
1	2	407	C

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Mol	Chain	Res	Type
1	2	415	G
1	2	421	C
1	2	423	U
1	2	424	C
1	2	425	U
1	2	426	G
1	2	437	U
1	2	440	G
1	2	449	A
1	2	456	C
1	2	458	G
1	2	459	G
1	2	460	A
1	2	462	U
1	2	464	A
1	2	470	G
1	2	474	A
1	2	483	G
1	2	484	G
1	2	485	C
1	2	487	G
1	2	490	G
1	2	493	G
1	2	497	U
1	2	498	A
1	2	499	A
1	2	501	A
1	2	513	A
1	2	519	G
1	2	527	U
1	2	530	U
1	2	531	U
1	2	532	G
1	2	539	A
1	2	542	C
1	2	543	G
1	2	551	C
1	2	571	C
1	2	595	G
1	2	600	G
1	2	609	A
1	2	620	U

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Mol	Chain	Res	Type
1	2	621	G
1	2	632	A
1	2	633	G
1	2	642	U
1	2	649	G
1	2	652	G
1	2	655	G
1	2	660	G
1	2	662	A
1	2	668	A
1	2	669	U
1	2	670	A
1	2	681	G
1	2	686	C
1	2	687	C
1	2	688	A
1	2	690	U
1	2	691	G
1	2	696	A
1	2	700	G
1	2	701	C
1	2	715	G
1	2	716	U
1	2	719	G
1	2	722	G
1	2	739	A
1	2	744	A
1	2	747	G
1	2	748	A
1	2	760	U
1	2	761	A
1	2	763	C
1	2	778	U
1	2	782	A
1	2	784	G
1	2	809	C
1	2	811	U
1	2	812	C
1	2	836	A
1	2	841	U
1	2	843	A
1	2	844	A

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Mol	Chain	Res	Type
1	2	856	G
1	2	861	G
1	2	871	A
1	2	873	G
1	2	885	A
1	2	897	G
1	2	905	C
1	2	908	C
1	2	915	U
1	2	920	C
1	2	928	U
1	2	932	U
1	2	939	5MC
1	2	940	A
1	2	941	A
1	2	942	C
1	2	943	G
1	2	946	G
1	2	947	G
1	2	949	A
1	2	950	A
1	2	953	U
1	2	964	G
1	2	965	A
1	2	966	C
1	2	967	G
1	2	968	G
1	2	974	U
1	2	975	G
1	2	976	A
1	2	977	A
1	2	978	G
1	2	980	C
1	2	990	G
1	2	991	G
1	2	996	G
1	2	997	C
1	2	999	G
1	2	1000	G
1	2	1001	A
1	2	1002	C
1	2	1004	C

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Mol	Chain	Res	Type
1	2	1005	G
1	2	1009	A
1	2	1018	G
1	2	1020	A
1	2	1029	G
1	2	1044	G
1	2	1054	C
1	2	1058	A
1	2	1059	G
1	2	1060	U
1	2	1066	A
1	2	1067	A
1	2	1092	G
1	2	1098	C
1	2	1103	C
1	2	1105	G
1	2	1106	C
1	2	1107	U
1	2	1108	C
1	2	1109	G
1	2	1114	G
1	2	1116	A
1	2	1120	A
1	2	1131	A
1	2	1133	U
1	2	1139	C
1	2	1145	G
1	2	1154	A
1	2	1156	G
1	2	1157	G
1	2	1158	G
1	2	1170	A
1	2	1171	G
1	2	1174	C
1	2	1186	A
1	2	1187	A
1	2	1199	A
1	2	1201	A
1	2	1202	5MC
1	2	1212	A
1	2	1213	A
1	2	1215	G

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Mol	Chain	Res	Type
1	2	1222	A
1	2	1230	U
1	2	1232	C
1	2	1236	C
1	2	1243	A
1	2	1244	G
1	2	1249	A
1	2	1252	U
1	2	1253	A
1	2	1254	A
1	2	1260	U
1	2	1261	A
1	2	1263	A
1	2	1264	C
1	2	1274	G
1	2	1276	U
1	2	1279	G
1	2	1282	C
1	2	1291	C
1	2	1294	C
1	2	1297	G
1	2	1300	C
1	2	1308	G
1	2	1309	C
1	2	1310	U
1	2	1312	G
1	2	1319	U
1	2	1327	G
1	2	1330	C
1	2	1336	C
1	2	1337	A
1	2	1338	U
1	2	1342	G
1	2	1344	G
1	2	1368	A
1	2	1371	C
1	2	1372	A
1	2	1374	C
1	2	1376	OMC
1	2	1388	C
1	2	1393	G
1	2	1394	C

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Mol	Chain	Res	Type
1	2	1398	G
1	2	1399	C
1	2	1400	C
1	2	1401	U
1	2	1424	G
1	2	1427	G
1	2	1428	G
1	2	1433	G
1	2	1436	G
1	2	1437	A
1	2	1442	A
1	2	1446	U
1	2	1452	A
1	2	1456	G
1	2	1461	A
1	2	1462	A
1	2	1463	G
1	2	1468	A
1	2	1471	A
1	2	1472	A
1	2	1473	G
1	2	1475	U
1	2	1476	A
1	2	1478	C
1	2	1486	G
1	2	1498	C
1	2	1499	G
30	5	813	A
30	5	814	U
30	5	815	U
30	5	816	U
30	5	818	A
30	5	822	C
30	5	823	C
31	4	3	C
31	4	6	G
31	4	7	G
31	4	8	4SU
31	4	9	G
31	4	14	A
31	4	15	G
31	4	16	C

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Mol	Chain	Res	Type
31	4	17	C
31	4	19	G
31	4	20	H2U
31	4	21	A
31	4	22	G
31	4	25	C
31	4	28	C
31	4	34	C
31	4	37	A
31	4	46	A
31	4	47	U
31	4	48	C
31	4	49	G
31	4	51	C
31	4	57	A
31	4	58	A
31	4	59	A
31	4	61	C
31	4	65	C
31	4	66	C
31	4	70	G
31	4	72	U
31	4	74	C
31	4	75	C
31	4	76	A

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	87	C
1	2	406	A
1	2	461	A
1	2	599	C
1	2	952	C
1	2	998	C
31	4	74	C

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

48 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	$\#\|Z\| > 2$
1	4AC	2	590	1	21,24,25	1.02	2 (9%)	29,34,37	1.34	4 (13%)
1	4AC	2	1193	1	21,24,25	1.12	3 (14%)	29,34,37	2.15	7 (24%)
1	4AC	2	718	1	21,24,25	0.99	2 (9%)	29,34,37	1.38	4 (13%)
1	4AC	2	851	1	21,24,25	1.16	1 (4%)	29,34,37	1.35	4 (13%)
1	4AC	2	1239	1	21,24,25	1.03	2 (9%)	29,34,37	1.48	3 (10%)
1	UR3	2	1467	1	19,22,23	0.99	2 (10%)	26,32,35	1.48	3 (11%)
1	5HM	2	1378	1	19,23,24	2.90	7 (36%)	25,33,36	0.79	0
1	4AC	2	1041	1	21,24,25	1.03	2 (9%)	29,34,37	1.26	4 (13%)
31	H2U	4	20	31	18,21,22	0.87	2 (11%)	21,30,33	1.72	2 (9%)
1	4AC	2	839	1	21,24,25	1.06	2 (9%)	29,34,37	1.38	4 (13%)
1	MA6	2	1488	1	18,26,27	0.85	0	19,38,41	1.29	2 (10%)
1	4AC	2	703	1	21,24,25	1.06	3 (14%)	29,34,37	1.53	5 (17%)
1	4AC	2	626	1	21,24,25	1.07	3 (14%)	29,34,37	1.38	4 (13%)
1	4AC	2	828	1	21,24,25	1.03	2 (9%)	29,34,37	1.32	5 (17%)
1	B8H	2	938	1	19,22,23	0.91	2 (10%)	22,32,35	1.48	2 (9%)
31	PSU	4	55	31	18,21,22	1.34	2 (11%)	22,30,33	2.00	4 (18%)
31	OMC	4	32	31	19,22,23	0.97	2 (10%)	26,31,34	0.89	1 (3%)
1	MA6	2	1487	1	18,26,27	0.83	0	19,38,41	1.22	2 (10%)
1	4AC	2	1184	1	21,24,25	1.03	2 (9%)	29,34,37	1.26	4 (13%)
1	4AC	2	319	1	21,24,25	1.04	2 (9%)	29,34,37	1.32	4 (13%)
1	4AC	2	1147	1	21,24,25	0.95	2 (9%)	29,34,37	1.32	4 (13%)
1	5MC	2	939	1	18,22,23	1.01	2 (11%)	26,32,35	1.30	4 (15%)
1	OMC	2	1376	1	19,22,23	0.99	2 (10%)	26,31,34	0.90	1 (3%)
1	4AC	2	1233	1	21,24,25	1.08	2 (9%)	29,34,37	1.47	4 (13%)
1	6MZ	2	1469	1,36	18,25,26	0.85	1 (5%)	16,36,39	2.04	3 (18%)
1	4AC	2	868	1	21,24,25	1.06	2 (9%)	29,34,37	1.25	4 (13%)
1	4AC	2	303	1	21,24,25	1.09	2 (9%)	29,34,37	1.40	4 (13%)
1	4AC	2	731	1	21,24,25	1.02	2 (9%)	29,34,37	1.15	3 (10%)
1	4AC	2	546	1	21,24,25	1.03	2 (9%)	29,34,37	1.26	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	4AC	2	1028	1	21,24,25	1.12	1 (4%)	29,34,37	1.37	4 (13%)
31	4SU	4	8	31	18,21,22	1.84	5 (27%)	26,30,33	2.15	6 (23%)
1	4AC	2	394	1	21,24,25	0.98	1 (4%)	29,34,37	1.60	5 (17%)
1	4AC	2	53	1	21,24,25	1.05	2 (9%)	29,34,37	1.34	4 (13%)
1	5MC	2	1202	1	18,22,23	0.97	1 (5%)	26,32,35	1.21	4 (15%)
1	LHH	2	250	1	22,25,26	2.61	8 (36%)	29,35,38	1.41	7 (24%)
31	5MU	4	54	31	19,22,23	1.43	5 (26%)	28,32,35	1.99	6 (21%)
1	4AC	2	379	1	21,24,25	1.04	2 (9%)	29,34,37	1.55	5 (17%)
1	4AC	2	648	1	21,24,25	1.04	2 (9%)	29,34,37	1.54	5 (17%)
1	4AC	2	1479	1	21,24,25	1.05	1 (4%)	29,34,37	1.22	2 (6%)
1	4AC	2	17	1	21,24,25	1.07	3 (14%)	29,34,37	1.47	5 (17%)
1	4AC	2	848	1	21,24,25	1.15	3 (14%)	29,34,37	1.24	3 (10%)
1	4AC	2	286	1	21,24,25	1.08	1 (4%)	29,34,37	1.52	4 (13%)
1	4AC	2	751	1	21,24,25	1.00	2 (9%)	29,34,37	1.25	4 (13%)
1	A2M	2	373	1	18,25,26	0.95	0	18,36,39	1.39	3 (16%)
1	4AC	2	511	1	21,24,25	1.02	2 (9%)	29,34,37	1.38	4 (13%)
1	4AC	2	957	1	21,24,25	1.16	2 (9%)	29,34,37	1.58	4 (13%)
1	4AC	2	479	1	21,24,25	1.05	2 (9%)	29,34,37	1.50	5 (17%)
1	4AC	2	636	1	21,24,25	1.08	2 (9%)	29,34,37	1.64	4 (13%)

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
1	4AC	2	590	1	-	0/11/29/30	0/2/2/2
1	4AC	2	1193	1	-	0/11/29/30	0/2/2/2
1	4AC	2	718	1	-	0/11/29/30	0/2/2/2
1	4AC	2	851	1	-	0/11/29/30	0/2/2/2
1	4AC	2	1239	1	-	2/11/29/30	0/2/2/2
1	UR3	2	1467	1	-	2/7/25/26	0/2/2/2
1	5HM	2	1378	1	-	2/9/27/28	0/2/2/2
1	4AC	2	1041	1	-	0/11/29/30	0/2/2/2
31	H2U	4	20	31	-	6/7/38/39	0/2/2/2
1	4AC	2	839	1	-	2/11/29/30	0/2/2/2
1	MA6	2	1488	1	-	0/7/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4AC	2	703	1	-	0/11/29/30	0/2/2/2
1	4AC	2	626	1	-	1/11/29/30	0/2/2/2
1	4AC	2	828	1	-	1/11/29/30	0/2/2/2
1	B8H	2	938	1	-	0/7/25/26	0/2/2/2
31	PSU	4	55	31	-	0/7/25/26	0/2/2/2
31	OMC	4	32	31	-	0/9/27/28	0/2/2/2
1	MA6	2	1487	1	-	0/7/29/30	0/3/3/3
1	4AC	2	1184	1	-	2/11/29/30	0/2/2/2
1	4AC	2	319	1	-	0/11/29/30	0/2/2/2
1	4AC	2	1147	1	-	1/11/29/30	0/2/2/2
1	5MC	2	939	1	-	2/7/25/26	0/2/2/2
1	OMC	2	1376	1	-	2/9/27/28	0/2/2/2
1	4AC	2	1233	1	-	0/11/29/30	0/2/2/2
1	6MZ	2	1469	1,36	-	0/5/27/28	0/3/3/3
1	4AC	2	868	1	-	1/11/29/30	0/2/2/2
1	4AC	2	303	1	-	1/11/29/30	0/2/2/2
1	4AC	2	731	1	-	0/11/29/30	0/2/2/2
1	4AC	2	546	1	-	2/11/29/30	0/2/2/2
1	4AC	2	1028	1	-	2/11/29/30	0/2/2/2
31	4SU	4	8	31	-	4/7/25/26	0/2/2/2
1	4AC	2	394	1	-	1/11/29/30	0/2/2/2
1	4AC	2	53	1	-	0/11/29/30	0/2/2/2
1	5MC	2	1202	1	-	3/7/25/26	0/2/2/2
1	LHH	2	250	1	-	1/13/31/32	0/2/2/2
31	5MU	4	54	31	-	1/7/25/26	0/2/2/2
1	4AC	2	379	1	-	3/11/29/30	0/2/2/2
1	4AC	2	648	1	-	2/11/29/30	0/2/2/2
1	4AC	2	1479	1	-	0/11/29/30	0/2/2/2
1	4AC	2	17	1	-	2/11/29/30	0/2/2/2
1	4AC	2	848	1	-	0/11/29/30	0/2/2/2
1	4AC	2	286	1	-	2/11/29/30	0/2/2/2
1	4AC	2	751	1	-	0/11/29/30	0/2/2/2
1	A2M	2	373	1	-	2/5/27/28	0/3/3/3
1	4AC	2	511	1	-	0/11/29/30	0/2/2/2
1	4AC	2	957	1	-	2/11/29/30	0/2/2/2
1	4AC	2	479	1	-	0/11/29/30	0/2/2/2
1	4AC	2	636	1	-	2/11/29/30	0/2/2/2

All (105) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	250	LHH	C4-N4	6.70	1.49	1.39
1	2	1378	5HM	C4-N3	6.12	1.44	1.34
1	2	250	LHH	C7-N4	6.07	1.48	1.37
1	2	1378	5HM	C2-N3	5.74	1.48	1.36
1	2	1378	5HM	C4-N4	5.44	1.48	1.34
1	2	1378	5HM	C6-C5	4.64	1.47	1.34
31	4	8	4SU	C4-S4	-4.46	1.59	1.68
1	2	250	LHH	O2-C2	-4.30	1.15	1.23
1	2	1378	5HM	C2-N1	3.79	1.48	1.40
1	2	851	4AC	C4-N3	-3.59	1.26	1.32
1	2	250	LHH	C2-N1	-3.59	1.32	1.40
31	4	8	4SU	C4-N3	-3.56	1.33	1.37
1	2	1028	4AC	C4-N3	-3.50	1.26	1.32
1	2	848	4AC	C4-N3	-3.32	1.27	1.32
1	2	1378	5HM	C6-N1	3.29	1.43	1.38
31	4	55	PSU	C6-C5	3.27	1.39	1.35
1	2	1202	5MC	C6-N1	-3.19	1.32	1.38
1	2	250	LHH	C6-N1	-3.16	1.30	1.38
1	2	1479	4AC	C4-N3	-3.07	1.27	1.32
1	2	1233	4AC	C4-N3	-3.04	1.27	1.32
1	2	1378	5HM	O2-C2	-3.04	1.18	1.23
1	2	957	4AC	C4-N3	-3.02	1.27	1.32
1	2	546	4AC	C4-N3	-2.95	1.27	1.32
1	2	53	4AC	C4-N3	-2.94	1.27	1.32
1	2	868	4AC	C4-N3	-2.92	1.27	1.32
1	2	731	4AC	C4-N3	-2.90	1.27	1.32
1	2	303	4AC	C4-N3	-2.90	1.27	1.32
1	2	17	4AC	C4-N3	-2.90	1.27	1.32
1	2	703	4AC	C4-N3	-2.90	1.27	1.32
1	2	1184	4AC	C4-N3	-2.87	1.27	1.32
1	2	319	4AC	C4-N3	-2.86	1.27	1.32
31	4	54	5MU	C4-N3	-2.85	1.33	1.38
1	2	590	4AC	C4-N3	-2.84	1.27	1.32
1	2	828	4AC	C4-N3	-2.84	1.27	1.32
1	2	479	4AC	C4-N3	-2.84	1.27	1.32
1	2	626	4AC	C4-N3	-2.83	1.27	1.32
1	2	636	4AC	C4-N3	-2.81	1.27	1.32
1	2	839	4AC	C4-N3	-2.80	1.27	1.32
31	4	8	4SU	C2-N1	2.78	1.42	1.38
1	2	1193	4AC	C4-N3	-2.75	1.28	1.32
1	2	250	LHH	C2-N3	-2.74	1.30	1.36
1	2	286	4AC	C4-N3	-2.74	1.28	1.32
31	4	54	5MU	C6-C5	2.74	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	939	5MC	C6-N1	-2.73	1.33	1.38
1	2	511	4AC	C4-N3	-2.73	1.28	1.32
1	2	1239	4AC	C4-N3	-2.72	1.28	1.32
1	2	1041	4AC	C4-N3	-2.71	1.28	1.32
1	2	939	5MC	C6-C5	2.69	1.39	1.34
1	2	379	4AC	C4-N3	-2.68	1.28	1.32
1	2	648	4AC	C4-N3	-2.68	1.28	1.32
1	2	751	4AC	C4-N3	-2.67	1.28	1.32
31	4	55	PSU	C4-N3	-2.63	1.34	1.38
1	2	957	4AC	C4-N4	-2.61	1.35	1.39
1	2	839	4AC	C5-C4	2.59	1.46	1.40
31	4	8	4SU	C5-C4	-2.57	1.39	1.42
1	2	394	4AC	C4-N3	-2.51	1.28	1.32
1	2	1467	UR3	C5-C4	-2.51	1.37	1.43
1	2	1041	4AC	C5-C4	2.49	1.46	1.40
1	2	828	4AC	C5-C4	2.47	1.46	1.40
1	2	718	4AC	C4-N3	-2.46	1.28	1.32
1	2	53	4AC	C5-C4	2.43	1.46	1.40
1	2	1376	OMC	C5-C4	-2.43	1.37	1.42
31	4	32	OMC	C5-C4	-2.43	1.37	1.42
1	2	1147	4AC	C5-C4	2.40	1.46	1.40
31	4	32	OMC	C6-N1	-2.40	1.32	1.38
1	2	731	4AC	C5-C4	2.38	1.45	1.40
1	2	1184	4AC	C5-C4	2.37	1.45	1.40
1	2	751	4AC	C5-C4	2.36	1.45	1.40
1	2	848	4AC	C4-N4	-2.35	1.36	1.39
31	4	20	H2U	C2-N3	-2.34	1.33	1.38
31	4	54	5MU	C2-N1	2.32	1.42	1.38
1	2	590	4AC	C5-C4	2.31	1.45	1.40
31	4	54	5MU	C6-N1	-2.31	1.34	1.38
1	2	938	B8H	C4-C5	-2.30	1.37	1.44
1	2	868	4AC	C5-C4	2.29	1.45	1.40
1	2	479	4AC	C5-C4	2.28	1.45	1.40
1	2	511	4AC	C5-C4	2.27	1.45	1.40
1	2	319	4AC	C5-C4	2.27	1.45	1.40
1	2	1193	4AC	C4-N4	-2.27	1.36	1.39
1	2	636	4AC	C4-N4	-2.27	1.36	1.39
1	2	718	4AC	C5-C4	2.27	1.45	1.40
1	2	848	4AC	C5-C4	2.27	1.45	1.40
1	2	648	4AC	C5-C4	2.26	1.45	1.40
1	2	1376	OMC	C6-N1	-2.26	1.32	1.38
1	2	546	4AC	C5-C4	2.25	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	4	8	4SU	C2-N3	-2.25	1.34	1.38
1	2	250	LHH	C6-C5	2.25	1.40	1.35
1	2	1467	UR3	C6-N1	-2.24	1.32	1.38
1	2	303	4AC	C4-N4	-2.24	1.36	1.39
1	2	379	4AC	C5-C4	2.23	1.45	1.40
1	2	1147	4AC	C4-N3	-2.23	1.28	1.32
1	2	250	LHH	O7-C7	-2.20	1.18	1.23
1	2	626	4AC	C5-C4	2.19	1.45	1.40
31	4	54	5MU	C2-N3	-2.18	1.34	1.38
1	2	1193	4AC	C6-C5	-2.15	1.30	1.35
31	4	20	H2U	C4-N3	-2.13	1.34	1.37
1	2	703	4AC	C5-C4	2.13	1.45	1.40
1	2	1233	4AC	C5-C4	2.13	1.45	1.40
1	2	1239	4AC	C5-C4	2.11	1.45	1.40
1	2	938	B8H	O4'-C1'	-2.09	1.40	1.43
1	2	17	4AC	C5-C4	2.08	1.45	1.40
1	2	1469	6MZ	C5-C4	2.08	1.46	1.40
1	2	703	4AC	C4-N4	-2.06	1.36	1.39
1	2	17	4AC	C4-N4	-2.04	1.36	1.39
1	2	626	4AC	C4-N4	-2.02	1.36	1.39

All (183) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	4	20	H2U	C4-N3-C2	-6.66	120.27	125.79
1	2	1469	6MZ	C2-N1-C6	6.24	121.94	116.59
31	4	55	PSU	N1-C2-N3	6.22	122.18	115.13
1	2	1193	4AC	O7-C7-N4	6.09	131.68	121.82
31	4	8	4SU	C4-N3-C2	-6.03	121.48	127.34
1	2	1467	UR3	C4-N3-C2	-5.75	119.15	124.56
1	2	1193	4AC	C5-C4-N4	-5.61	113.18	122.92
1	2	1193	4AC	N4-C4-N3	5.46	123.02	113.85
31	4	8	4SU	C5-C4-N3	5.40	119.69	114.69
1	2	636	4AC	O7-C7-N4	5.28	130.37	121.82
1	2	938	B8H	C4-N3-C2	-5.27	120.53	127.35
1	2	957	4AC	O7-C7-N4	5.22	130.27	121.82
31	4	54	5MU	N3-C2-N1	5.04	121.58	114.89
1	2	394	4AC	O7-C7-N4	4.99	129.90	121.82
1	2	319	4AC	O7-C7-N4	4.98	129.87	121.82
1	2	1233	4AC	O7-C7-N4	4.77	129.54	121.82
1	2	703	4AC	O7-C7-N4	4.73	129.47	121.82
1	2	1028	4AC	O7-C7-N4	4.70	129.43	121.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	303	4AC	O7-C7-N4	4.68	129.39	121.82
1	2	839	4AC	O7-C7-N4	4.68	129.39	121.82
31	4	54	5MU	C4-N3-C2	-4.64	121.34	127.35
1	2	626	4AC	O7-C7-N4	4.61	129.28	121.82
1	2	648	4AC	O7-C7-N4	4.60	129.27	121.82
1	2	17	4AC	O7-C7-N4	4.52	129.13	121.82
1	2	590	4AC	O7-C7-N4	4.49	129.09	121.82
1	2	286	4AC	O7-C7-N4	4.47	129.04	121.82
1	2	479	4AC	O7-C7-N4	4.46	129.04	121.82
1	2	1239	4AC	O7-C7-N4	4.45	129.02	121.82
1	2	53	4AC	O7-C7-N4	4.45	129.01	121.82
1	2	1184	4AC	O7-C7-N4	4.44	129.01	121.82
1	2	851	4AC	O7-C7-N4	4.37	128.88	121.82
1	2	828	4AC	O7-C7-N4	4.36	128.88	121.82
1	2	718	4AC	O7-C7-N4	4.35	128.87	121.82
1	2	511	4AC	O7-C7-N4	4.34	128.84	121.82
1	2	1041	4AC	O7-C7-N4	4.27	128.73	121.82
1	2	546	4AC	O7-C7-N4	4.23	128.66	121.82
1	2	379	4AC	O7-C7-N4	4.23	128.66	121.82
1	2	1147	4AC	O7-C7-N4	4.22	128.64	121.82
1	2	751	4AC	O7-C7-N4	4.21	128.63	121.82
1	2	868	4AC	O7-C7-N4	4.08	128.42	121.82
1	2	1479	4AC	O7-C7-N4	4.08	128.41	121.82
31	4	55	PSU	C4-N3-C2	-4.07	120.47	126.34
1	2	636	4AC	C5-C4-N4	-4.05	115.89	122.92
1	2	731	4AC	O7-C7-N4	4.02	128.33	121.82
31	4	8	4SU	N3-C2-N1	3.97	120.17	114.89
31	4	54	5MU	O4-C4-C5	-3.94	120.34	124.90
1	2	848	4AC	O7-C7-N4	3.91	128.14	121.82
31	4	54	5MU	C5-C4-N3	3.90	118.64	115.31
1	2	379	4AC	N4-C4-N3	3.79	120.22	113.85
31	4	8	4SU	C1'-N1-C2	3.74	124.35	117.57
1	2	1488	MA6	N3-C2-N1	-3.72	122.86	128.68
1	2	1469	6MZ	C4-C5-N7	-3.69	105.56	109.40
31	4	55	PSU	O2-C2-N1	-3.66	118.76	122.79
1	2	286	4AC	N4-C4-N3	3.66	119.99	113.85
1	2	394	4AC	N4-C4-N3	3.66	119.99	113.85
1	2	939	5MC	C5-C6-N1	-3.64	119.59	123.34
1	2	1239	4AC	N4-C4-N3	3.55	119.81	113.85
1	2	379	4AC	C5-C4-N4	-3.53	116.78	122.92
1	2	1239	4AC	C5-C4-N4	-3.52	116.80	122.92
1	2	1487	MA6	C4-C5-N7	-3.50	105.75	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	636	4AC	N4-C4-N3	3.49	119.72	113.85
1	2	648	4AC	C5-C4-N4	-3.46	116.91	122.92
1	2	703	4AC	C5-C4-N4	-3.44	116.95	122.92
1	2	286	4AC	C5-C4-N4	-3.41	116.99	122.92
1	2	718	4AC	C5-C4-N4	-3.40	117.01	122.92
1	2	957	4AC	C5-C4-N4	-3.34	117.12	122.92
1	2	636	4AC	CM7-C7-N4	-3.32	109.56	115.29
1	2	394	4AC	C5-C4-N4	-3.31	117.17	122.92
1	2	648	4AC	N4-C4-N3	3.30	119.39	113.85
1	2	703	4AC	N4-C4-N3	3.29	119.37	113.85
1	2	479	4AC	CM7-C7-N4	-3.24	109.69	115.29
1	2	303	4AC	C5-C4-N4	-3.24	117.30	122.92
1	2	1233	4AC	N4-C4-N3	3.23	119.27	113.85
1	2	957	4AC	CM7-C7-N4	-3.21	109.74	115.29
1	2	1202	5MC	C5-C6-N1	-3.18	120.06	123.34
1	2	1469	6MZ	N3-C2-N1	-3.17	123.72	128.68
1	2	626	4AC	N4-C4-N3	3.16	119.16	113.85
1	2	373	A2M	N3-C2-N1	-3.16	123.74	128.68
1	2	511	4AC	N4-C4-N3	3.14	119.12	113.85
1	2	1487	MA6	N3-C2-N1	-3.13	123.79	128.68
1	2	1233	4AC	C5-C4-N4	-3.12	117.49	122.92
1	2	1488	MA6	C4-C5-N7	-3.06	106.21	109.40
1	2	250	LHH	CM7-C7-N4	3.05	120.57	115.29
1	2	511	4AC	C5-C4-N4	-3.04	117.64	122.92
1	2	718	4AC	N4-C4-N3	3.01	118.91	113.85
1	2	303	4AC	N4-C4-N3	3.01	118.91	113.85
1	2	1147	4AC	N4-C4-N3	3.01	118.90	113.85
1	2	626	4AC	C5-C4-N4	-2.99	117.73	122.92
1	2	479	4AC	C5-C4-N4	-2.93	117.82	122.92
1	2	53	4AC	CM7-C7-N4	-2.92	110.24	115.29
1	2	590	4AC	N4-C4-N3	2.88	118.68	113.85
1	2	17	4AC	C5-C4-N4	-2.85	117.97	122.92
1	2	1028	4AC	N4-C4-N3	2.83	118.60	113.85
1	2	17	4AC	CM7-C7-N4	-2.83	110.40	115.29
1	2	479	4AC	N4-C4-N3	2.82	118.58	113.85
1	2	17	4AC	N4-C4-N3	2.82	118.58	113.85
1	2	250	LHH	C5-C4-N3	-2.82	118.06	122.59
1	2	1028	4AC	C5-C4-N4	-2.81	118.03	122.92
1	2	718	4AC	CM7-C7-N4	-2.79	110.47	115.29
31	4	54	5MU	C5-C6-N1	-2.78	120.48	123.34
1	2	848	4AC	CM7-C7-N4	-2.77	110.50	115.29
31	4	8	4SU	C5-C4-S4	-2.77	120.90	124.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	839	4AC	C5-C4-N4	-2.76	118.13	122.92
1	2	839	4AC	N4-C4-N3	2.74	118.45	113.85
1	2	1041	4AC	CM7-C7-N4	-2.73	110.57	115.29
1	2	1147	4AC	C5-C4-N4	-2.73	118.18	122.92
1	2	703	4AC	CM7-C7-N4	-2.72	110.58	115.29
1	2	1479	4AC	CM7-C7-N4	-2.71	110.60	115.29
1	2	546	4AC	CM7-C7-N4	-2.70	110.62	115.29
1	2	939	5MC	C5-C4-N3	-2.70	118.76	121.67
1	2	394	4AC	CM7-C7-N4	-2.70	110.63	115.29
1	2	303	4AC	CM7-C7-N4	-2.69	110.65	115.29
1	2	1233	4AC	CM7-C7-N4	-2.67	110.68	115.29
1	2	1202	5MC	O2-C2-N3	-2.67	118.00	122.33
1	2	373	A2M	C4-C5-N7	-2.65	106.64	109.40
1	2	590	4AC	CM7-C7-N4	-2.65	110.71	115.29
1	2	648	4AC	CM7-C7-N4	-2.65	110.71	115.29
1	2	546	4AC	N4-C4-N3	2.65	118.30	113.85
1	2	939	5MC	O2-C2-N3	-2.65	118.03	122.33
1	2	590	4AC	C5-C4-N4	-2.64	118.33	122.92
1	2	751	4AC	C5-C4-N4	-2.63	118.35	122.92
1	2	751	4AC	CM7-C7-N4	-2.61	110.78	115.29
1	2	938	B8H	N3-C2-N1	2.61	117.96	115.14
1	2	53	4AC	N4-C4-N3	2.59	118.19	113.85
1	2	957	4AC	N4-C4-N3	2.58	118.19	113.85
1	2	479	4AC	O2-C2-N3	-2.56	118.16	122.33
1	2	53	4AC	C5-C4-N4	-2.55	118.49	122.92
1	2	868	4AC	CM7-C7-N4	-2.55	110.89	115.29
1	2	626	4AC	CM7-C7-N4	-2.54	110.89	115.29
1	2	1193	4AC	O7-C7-CM7	-2.54	117.35	122.06
1	2	250	LHH	C5-C6-N1	-2.52	117.58	121.81
1	2	828	4AC	N4-C4-N3	2.52	118.08	113.85
1	2	1193	4AC	C1'-N1-C2	2.51	124.03	118.42
1	2	250	LHH	N4-C4-N3	2.51	118.07	113.85
1	2	731	4AC	CM7-C7-N4	-2.51	110.96	115.29
1	2	1193	4AC	CM7-C7-N4	-2.50	110.97	115.29
31	4	8	4SU	O2-C2-N3	-2.50	116.85	121.50
1	2	17	4AC	O2-C2-N3	-2.47	118.31	122.33
31	4	54	5MU	C1'-N1-C2	2.46	122.03	117.57
1	2	319	4AC	N4-C4-N3	2.43	117.93	113.85
1	2	1041	4AC	C5-C4-N4	-2.43	118.70	122.92
1	2	868	4AC	N4-C4-N3	2.43	117.93	113.85
1	2	868	4AC	C5-C4-N4	-2.43	118.70	122.92
1	2	511	4AC	CM7-C7-N4	-2.43	111.10	115.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1028	4AC	CM7-C7-N4	-2.40	111.14	115.29
1	2	751	4AC	N4-C4-N3	2.40	117.88	113.85
1	2	828	4AC	CM7-C7-N4	-2.40	111.15	115.29
1	2	394	4AC	C1'-N1-C2	2.39	123.75	118.42
1	2	1467	UR3	C1'-N1-C2	2.38	121.01	116.99
1	2	319	4AC	CM7-C7-N4	-2.37	111.20	115.29
1	2	828	4AC	C5-C4-N4	-2.36	118.82	122.92
1	2	1184	4AC	C5-C4-N4	-2.36	118.82	122.92
1	2	839	4AC	CM7-C7-N4	-2.36	111.22	115.29
1	2	286	4AC	CM7-C7-N4	-2.31	111.29	115.29
1	2	373	A2M	O2'-C2'-C1'	-2.31	104.52	109.09
1	2	851	4AC	N4-C4-N3	2.31	117.72	113.85
1	2	1041	4AC	N4-C4-N3	2.30	117.71	113.85
31	4	55	PSU	C5-C6-N1	-2.29	118.68	122.11
1	2	379	4AC	C1'-N1-C2	2.27	123.50	118.42
1	2	848	4AC	C5-C4-N4	-2.25	119.01	122.92
1	2	1184	4AC	N4-C4-N3	2.24	117.61	113.85
1	2	1376	OMC	O2-C2-N3	-2.23	118.70	122.33
1	2	250	LHH	C6-C5-C4	2.22	119.68	116.96
31	4	32	OMC	O2-C2-N3	-2.21	118.74	122.33
1	2	1147	4AC	CM7-C7-N4	-2.20	111.49	115.29
1	2	851	4AC	C1'-N1-C6	2.18	125.59	120.84
1	2	1202	5MC	C5-C4-N3	-2.17	119.33	121.67
1	2	319	4AC	C5-C4-N4	-2.17	119.15	122.92
1	2	250	LHH	O7-C7-CM7	-2.16	118.04	122.06
1	2	250	LHH	N1-C2-N3	2.16	122.75	118.81
1	2	939	5MC	N1-C2-N3	2.14	122.71	118.81
1	2	1202	5MC	C1'-N1-C6	-2.13	117.57	121.12
1	2	1467	UR3	C3U-N3-C4	2.12	120.91	117.89
1	2	546	4AC	C5-C4-N4	-2.11	119.25	122.92
1	2	851	4AC	C5-C4-N4	-2.10	119.27	122.92
1	2	731	4AC	O2-C2-N3	-2.08	118.94	122.33
1	2	828	4AC	O2-C2-N3	-2.06	118.98	122.33
1	2	648	4AC	O2-C2-N3	-2.06	118.98	122.33
1	2	379	4AC	O2-C2-N3	-2.06	118.99	122.33
1	2	703	4AC	O2-C2-N3	-2.02	119.04	122.33
1	2	1184	4AC	CM7-C7-N4	-2.02	111.80	115.29
1	2	1193	4AC	C1'-N1-C6	-2.02	116.44	120.84
31	4	20	H2U	O4-C4-N3	2.00	123.46	120.28

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	250	LHH	C1'-C2'-O2'-C1
1	2	286	4AC	O4'-C4'-C5'-O5'
1	2	286	4AC	C3'-C4'-C5'-O5'
1	2	546	4AC	O4'-C4'-C5'-O5'
1	2	546	4AC	C3'-C4'-C5'-O5'
1	2	636	4AC	O4'-C4'-C5'-O5'
1	2	636	4AC	C3'-C4'-C5'-O5'
1	2	839	4AC	O4'-C4'-C5'-O5'
1	2	939	5MC	O4'-C4'-C5'-O5'
1	2	939	5MC	C3'-C4'-C5'-O5'
1	2	957	4AC	O4'-C4'-C5'-O5'
1	2	957	4AC	C3'-C4'-C5'-O5'
1	2	1028	4AC	O4'-C4'-C5'-O5'
1	2	1028	4AC	C3'-C4'-C5'-O5'
1	2	1202	5MC	O4'-C4'-C5'-O5'
1	2	1202	5MC	C3'-C4'-C5'-O5'
1	2	1376	OMC	C3'-C4'-C5'-O5'
1	2	1378	5HM	C6-C5-CM5-OM5
1	2	1378	5HM	C4-C5-CM5-OM5
31	4	8	4SU	O4'-C4'-C5'-O5'
1	2	373	A2M	O4'-C4'-C5'-O5'
1	2	373	A2M	C3'-C4'-C5'-O5'
1	2	839	4AC	C3'-C4'-C5'-O5'
1	2	1184	4AC	O4'-C4'-C5'-O5'
1	2	1239	4AC	C3'-C4'-C5'-O5'
1	2	1376	OMC	O4'-C4'-C5'-O5'
31	4	8	4SU	C3'-C4'-C5'-O5'
31	4	20	H2U	C2'-C1'-N1-C2
1	2	1239	4AC	O4'-C4'-C5'-O5'
1	2	1467	UR3	O4'-C4'-C5'-O5'
31	4	20	H2U	C2'-C1'-N1-C6
1	2	379	4AC	C3'-C4'-C5'-O5'
1	2	648	4AC	C3'-C4'-C5'-O5'
1	2	1184	4AC	C3'-C4'-C5'-O5'
1	2	1467	UR3	C3'-C4'-C5'-O5'
1	2	379	4AC	O4'-C4'-C5'-O5'
1	2	648	4AC	O4'-C4'-C5'-O5'
1	2	828	4AC	O4'-C4'-C5'-O5'
31	4	20	H2U	C3'-C4'-C5'-O5'
1	2	868	4AC	C3'-C4'-C5'-O5'
1	2	1147	4AC	C3'-C4'-C5'-O5'
31	4	8	4SU	C2'-C1'-N1-C2
31	4	8	4SU	C2'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
31	4	20	H2U	O4'-C1'-N1-C2
1	2	17	4AC	C3'-C4'-C5'-O5'
1	2	303	4AC	O4'-C4'-C5'-O5'
31	4	20	H2U	O4'-C4'-C5'-O5'
1	2	17	4AC	C2'-C1'-N1-C2
31	4	20	H2U	C4'-C5'-O5'-P
1	2	379	4AC	C2'-C1'-N1-C2
1	2	394	4AC	C2'-C1'-N1-C2
31	4	54	5MU	C2'-C1'-N1-C2
1	2	626	4AC	O4'-C4'-C5'-O5'
1	2	1202	5MC	C2'-C1'-N1-C2

There are no ring outliers.

34 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	1193	4AC	2	0
1	2	718	4AC	1	0
1	2	1239	4AC	3	0
1	2	1467	UR3	1	0
1	2	1378	5HM	2	0
1	2	1041	4AC	1	0
31	4	20	H2U	1	0
1	2	839	4AC	1	0
1	2	1488	MA6	1	0
1	2	703	4AC	4	0
1	2	626	4AC	1	0
31	4	55	PSU	2	0
1	2	1487	MA6	1	0
1	2	1184	4AC	2	0
1	2	1147	4AC	1	0
1	2	1233	4AC	1	0
1	2	868	4AC	1	0
1	2	303	4AC	1	0
1	2	1028	4AC	1	0
31	4	8	4SU	3	0
1	2	394	4AC	1	0
1	2	53	4AC	1	0
31	4	54	5MU	1	0
1	2	379	4AC	1	0
1	2	648	4AC	1	0
1	2	17	4AC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	848	4AC	2	0
1	2	286	4AC	3	0
1	2	751	4AC	1	0
1	2	373	A2M	1	0
1	2	511	4AC	2	0
1	2	957	4AC	1	0
1	2	479	4AC	2	0
1	2	636	4AC	3	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 42 ligands modelled in this entry, 40 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
38	MET	4	101	-	6,7,8	0.46	0	2,7,9	0.14	0
39	GNP	7	501	36	29,34,34	1.63	7 (24%)	33,54,54	2.15	6 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	MET	4	101	-	-	2/5/6/8	-
39	GNP	7	501	36	-	6/14/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	7	501	GNP	PB-O3A	4.38	1.64	1.59
39	7	501	GNP	PG-N3B	3.13	1.71	1.63
39	7	501	GNP	C6-N1	3.10	1.38	1.33
39	7	501	GNP	PB-O1B	3.06	1.51	1.46
39	7	501	GNP	PG-O1G	2.56	1.50	1.46
39	7	501	GNP	PB-O2B	-2.27	1.50	1.56
39	7	501	GNP	C5-C6	2.07	1.44	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	7	501	GNP	C5-C6-N1	-8.44	111.89	123.43
39	7	501	GNP	C2-N1-C6	5.82	125.18	115.93
39	7	501	GNP	PB-O3A-PA	-2.93	122.28	132.62
39	7	501	GNP	N3-C2-N1	-2.79	123.50	127.22
39	7	501	GNP	C4-C5-C6	-2.61	118.31	120.80
39	7	501	GNP	C2-N3-C4	-2.19	112.86	115.36

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
39	7	501	GNP	PB-N3B-PG-O1G
39	7	501	GNP	PG-N3B-PB-O1B
39	7	501	GNP	C5'-O5'-PA-O1A
39	7	501	GNP	C5'-O5'-PA-O2A
38	4	101	MET	CA-CB-CG-SD
38	4	101	MET	CB-CG-SD-CE
39	7	501	GNP	C5'-O5'-PA-O3A
39	7	501	GNP	C4'-C5'-O5'-PA

There are no ring outliers.

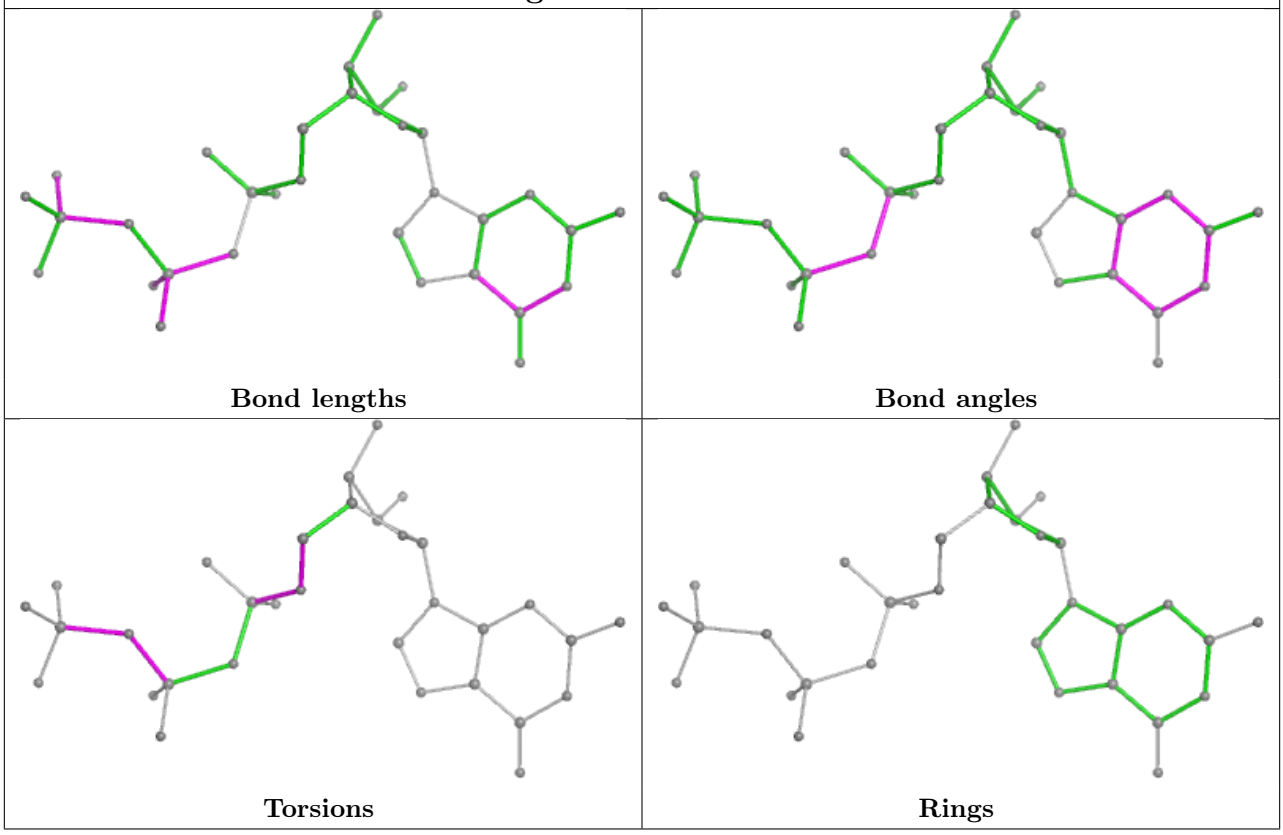
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	4	101	MET	4	0
39	7	501	GNP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GNP 7 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

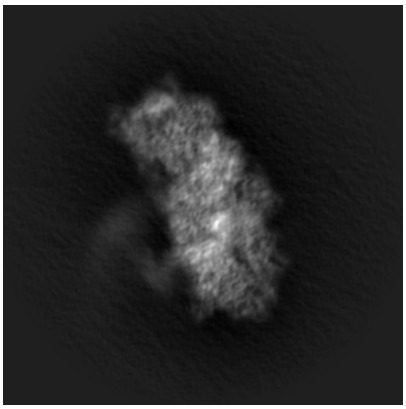
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10322. These allow visual inspection of the internal detail of the map and identification of artifacts.

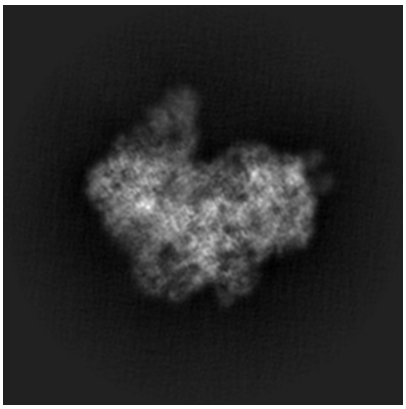
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

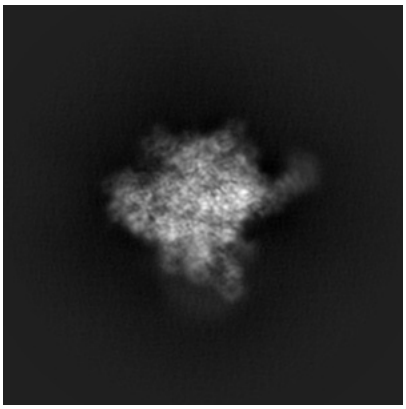
6.1.1 Primary map



X

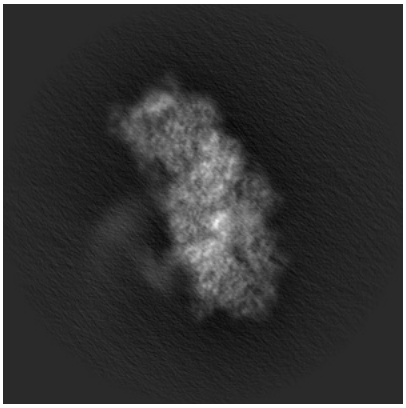


Y

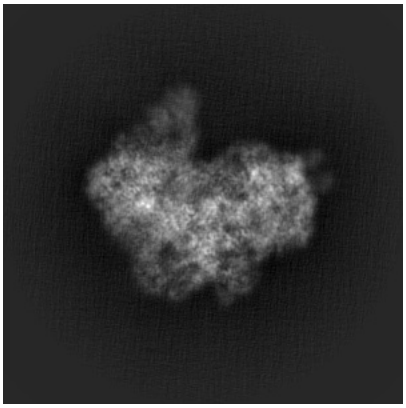


Z

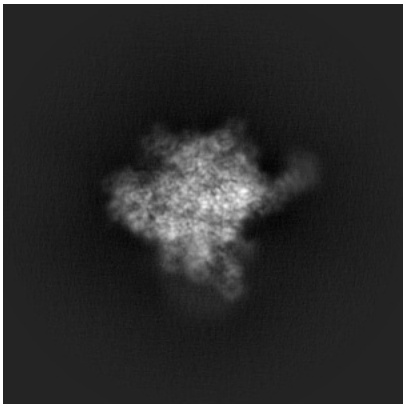
6.1.2 Raw map



X



Y

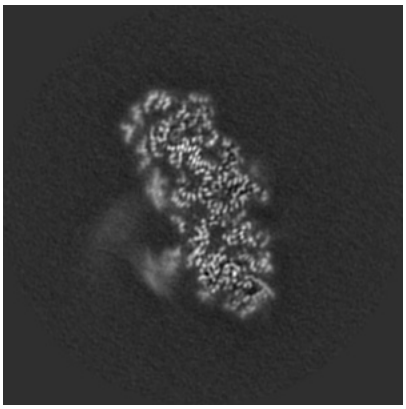


Z

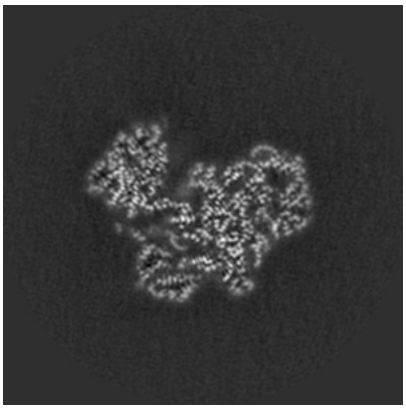
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

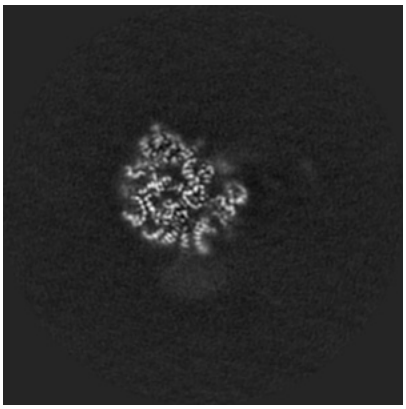
6.2.1 Primary map



X Index: 174

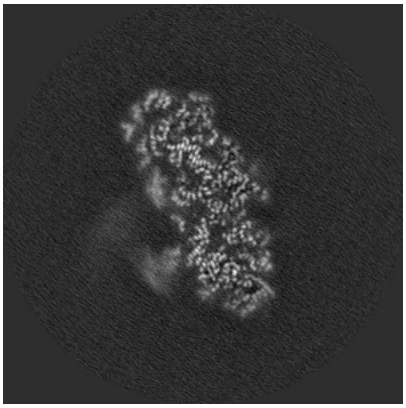


Y Index: 174

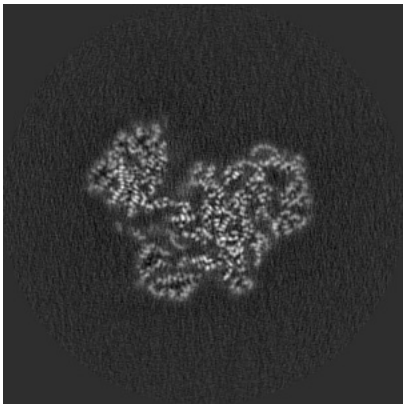


Z Index: 174

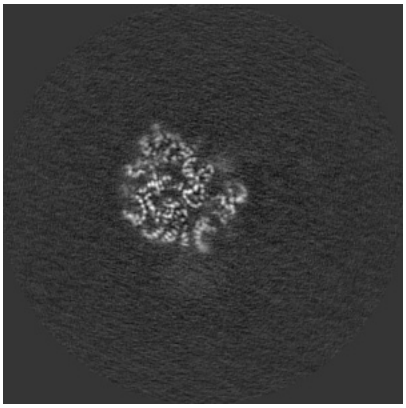
6.2.2 Raw map



X Index: 174



Y Index: 174

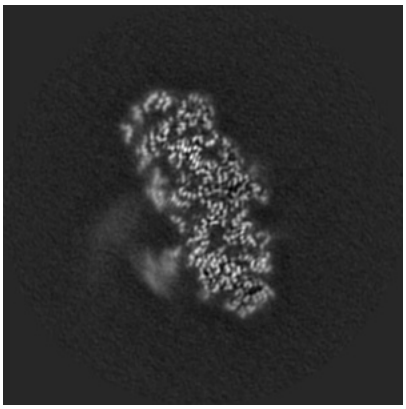


Z Index: 174

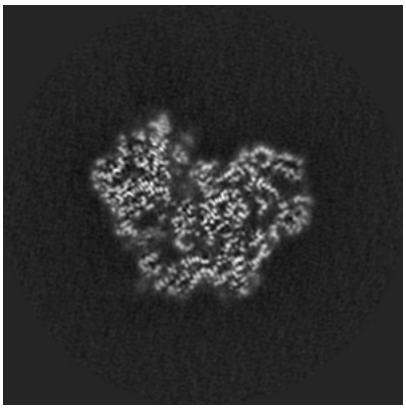
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

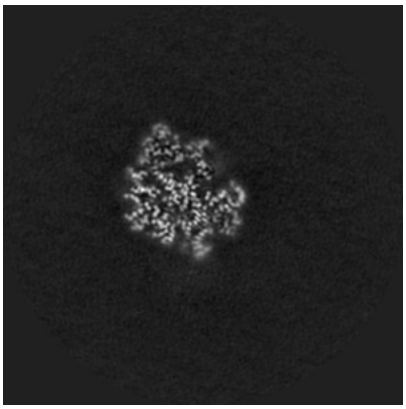
6.3.1 Primary map



X Index: 173

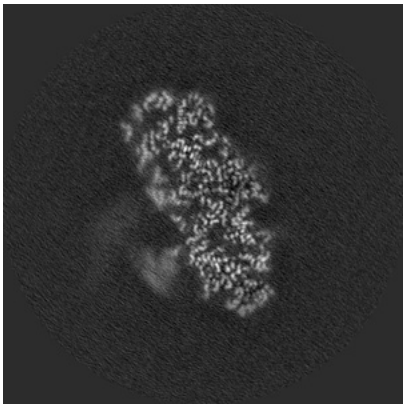


Y Index: 179

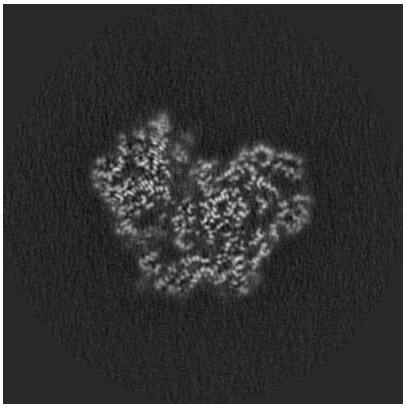


Z Index: 180

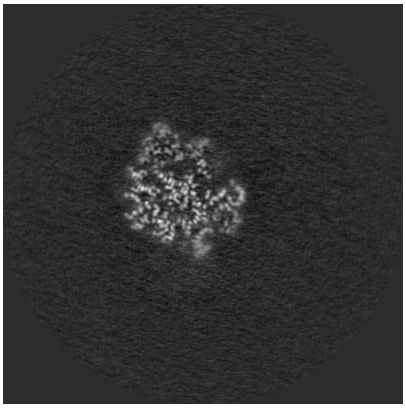
6.3.2 Raw map



X Index: 172



Y Index: 179

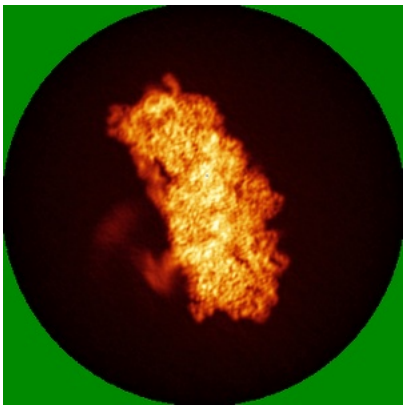


Z Index: 180

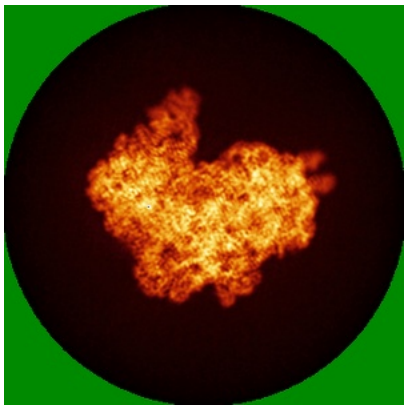
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

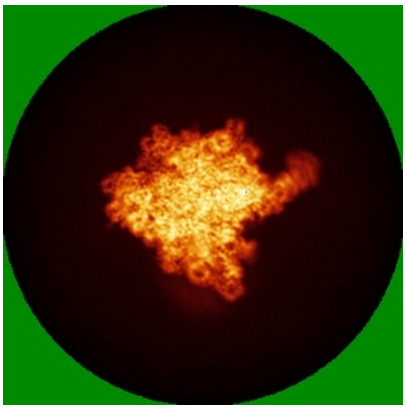
6.4.1 Primary map



X

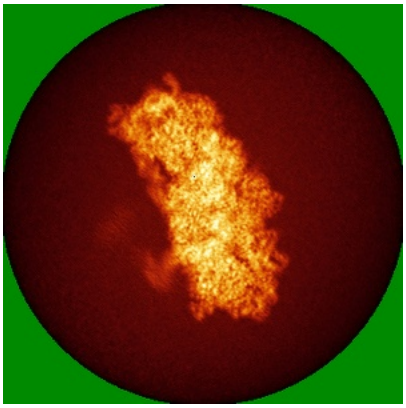


Y

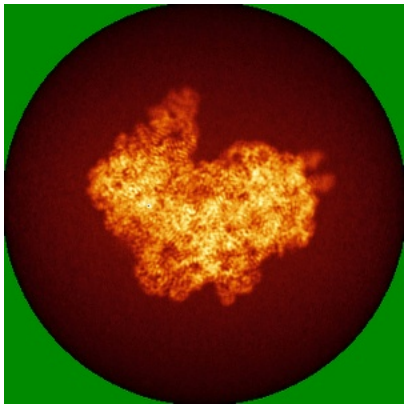


Z

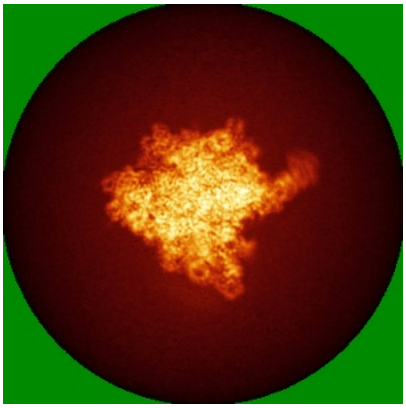
6.4.2 Raw map



X



Y



Z

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

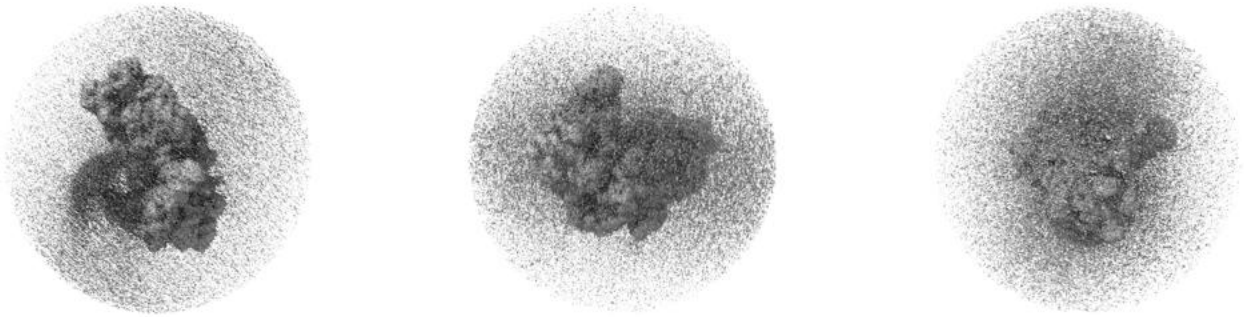
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.003. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

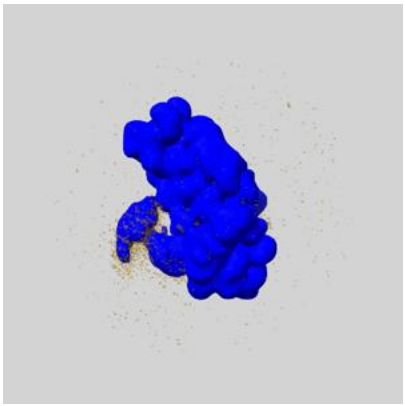
6.6 Mask visualisation (i)

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

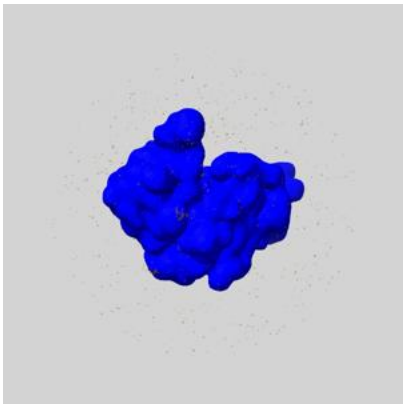
A mask typically either:

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

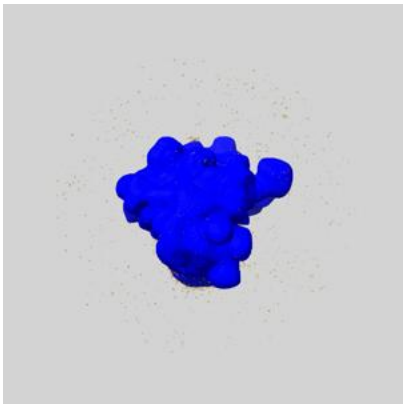
6.6.1 emd_10322_msk_1.map (i)



X



Y

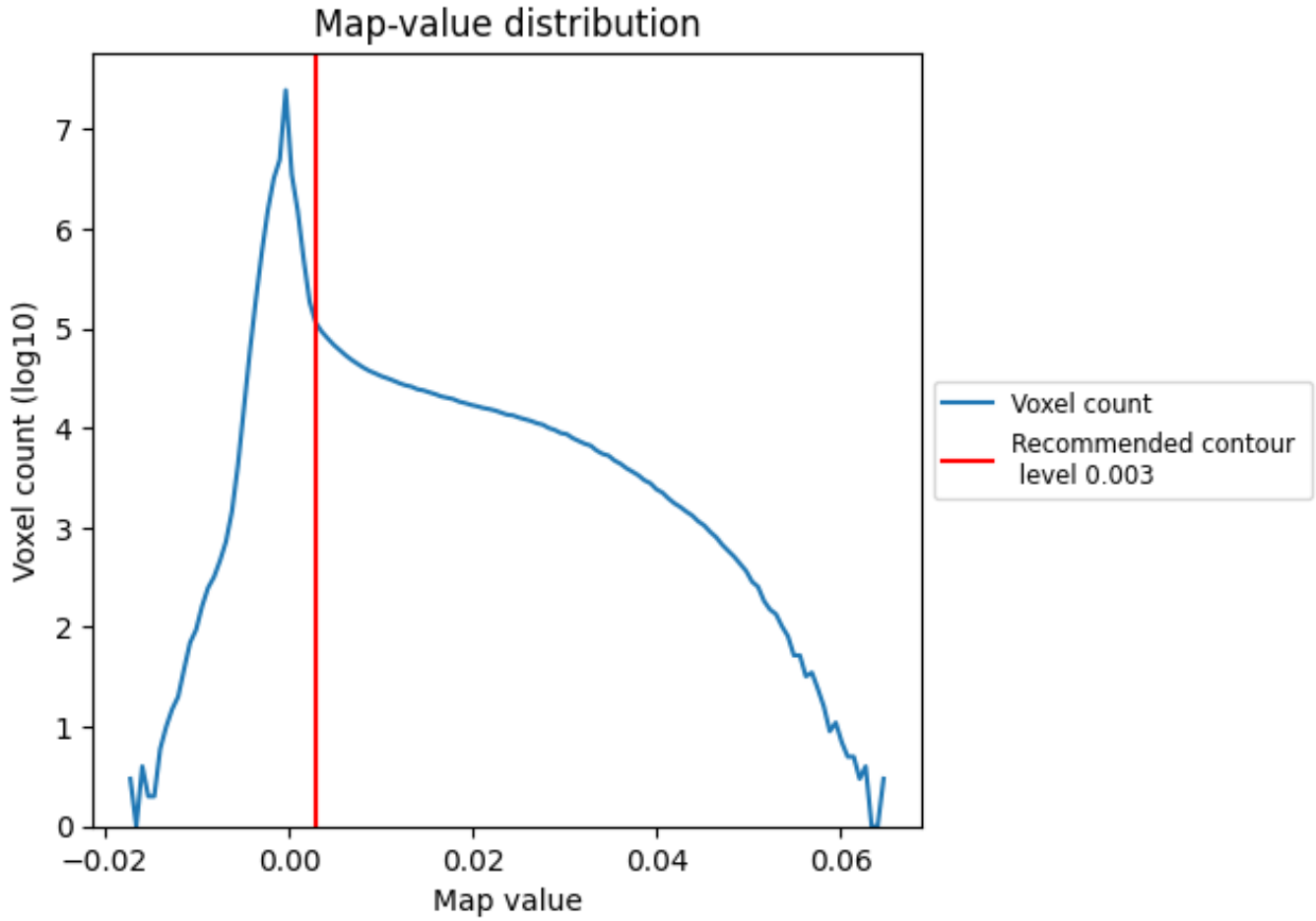


Z

7 Map analysis

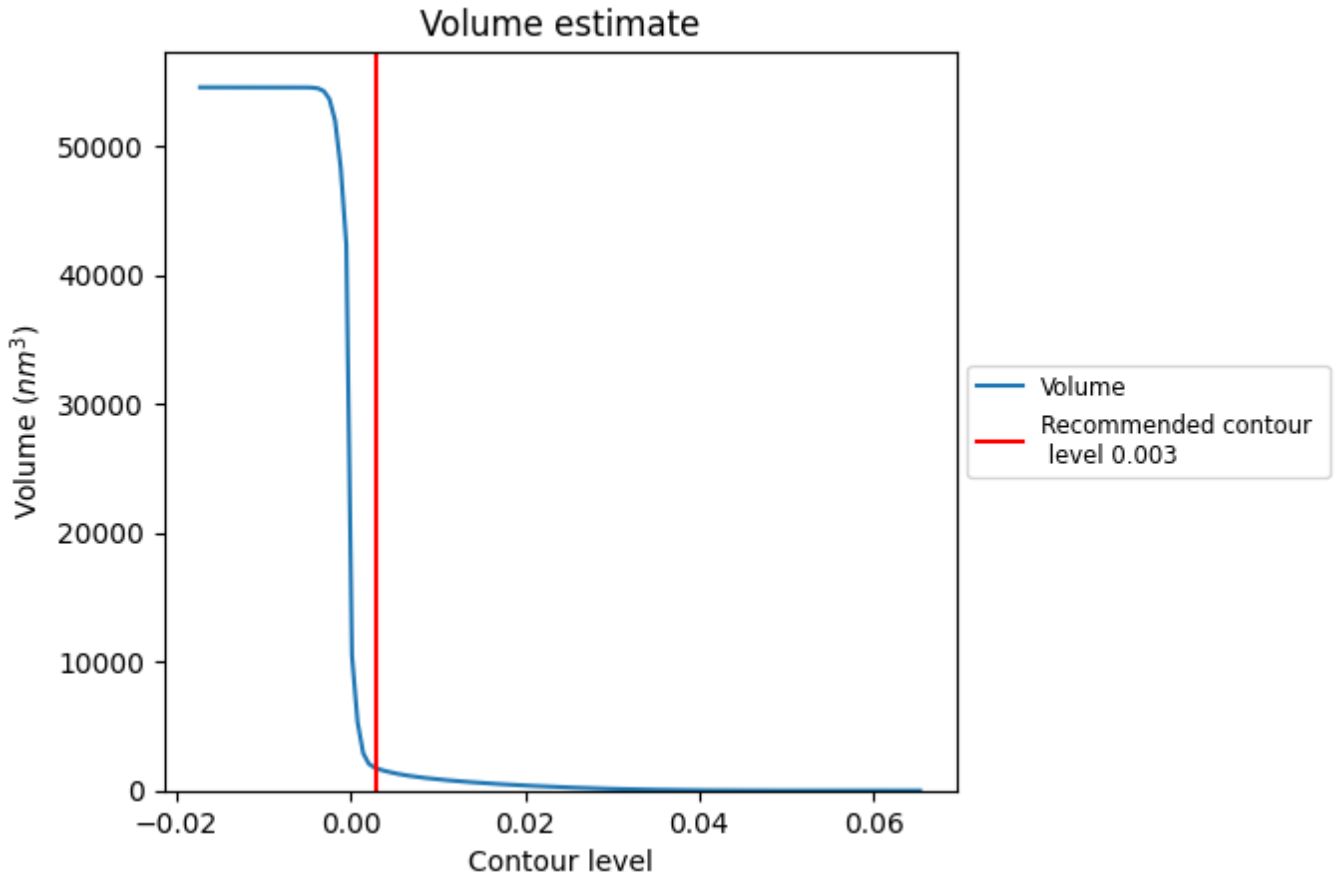
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

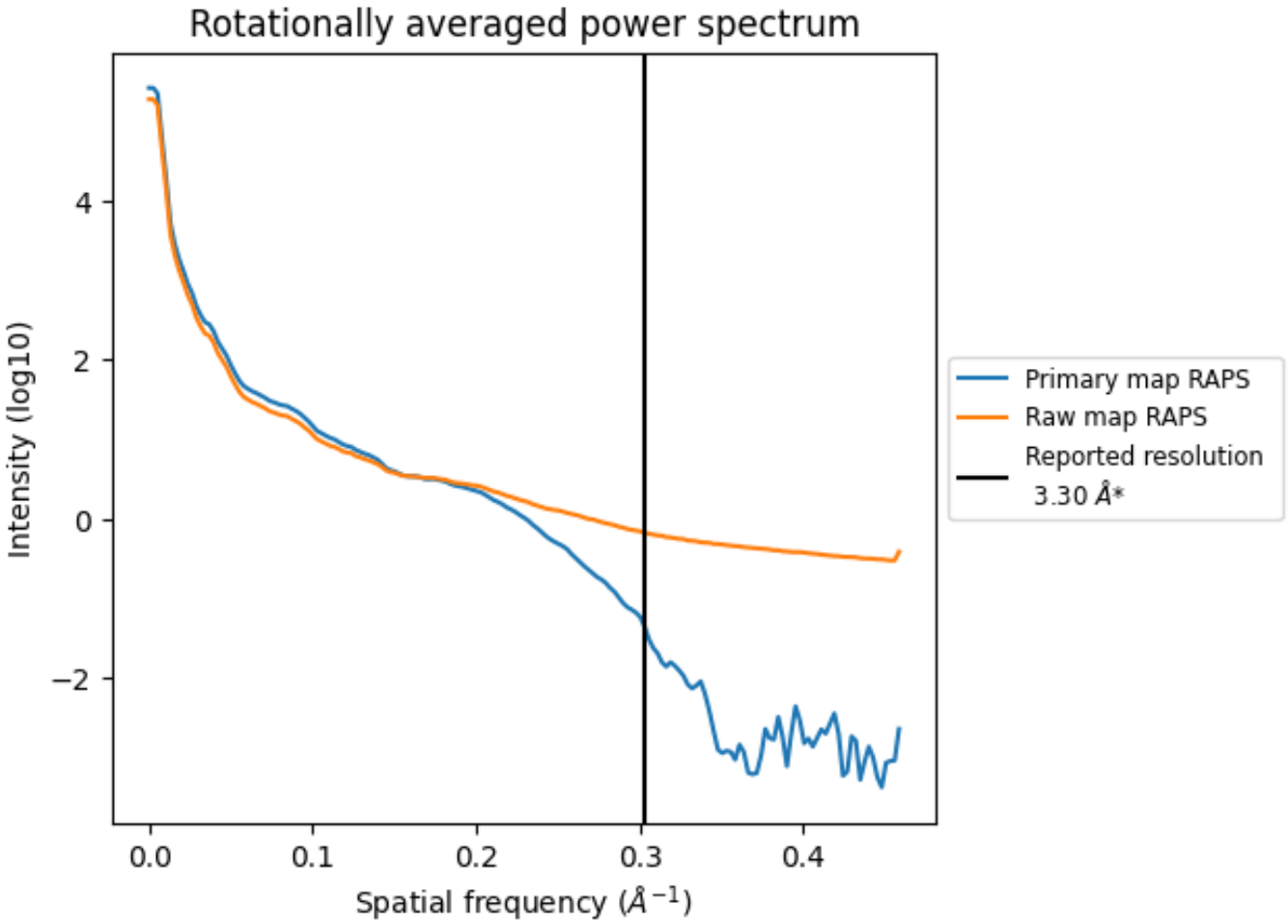
7.2 Volume estimate



The volume at the recommended contour level is 1725 nm^3; this corresponds to an approximate mass of 1559 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 (i)

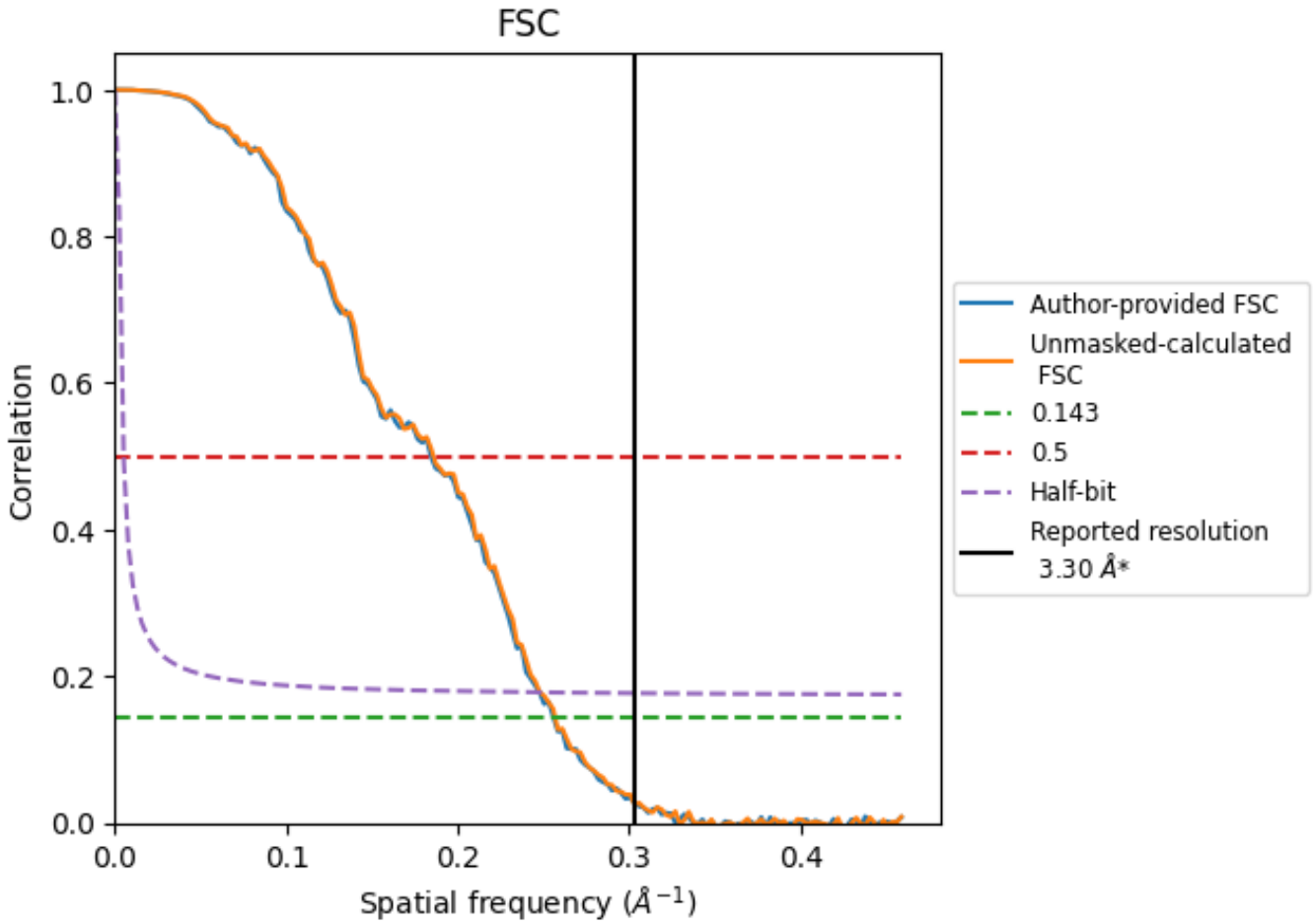


*Reported resolution corresponds to spatial frequency of 0.303 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.91	5.42	4.04
Unmasked-calculated*	3.89	5.38	4.03

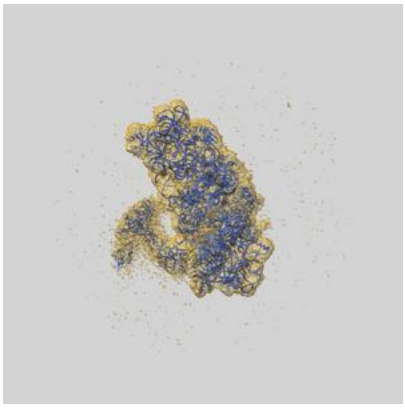
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.91 differs from the reported value 3.3 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.89 differs from the reported value 3.3 by more than 10 %

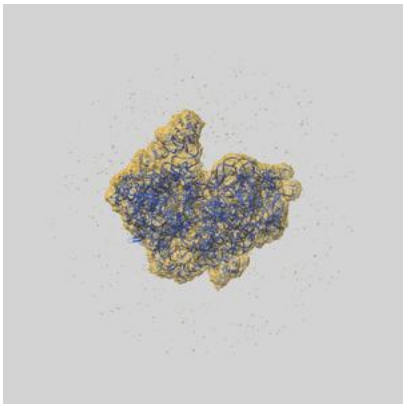
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10322 and PDB model 6SWC. Per-residue inclusion information can be found in section 3 on page 13.

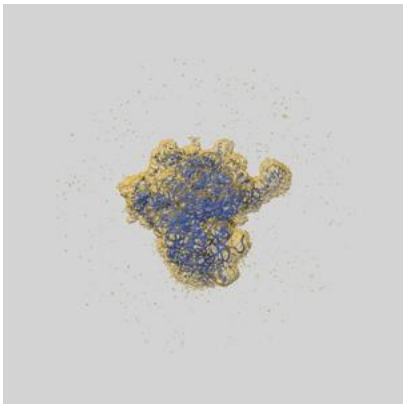
9.1 Map-model overlay



X



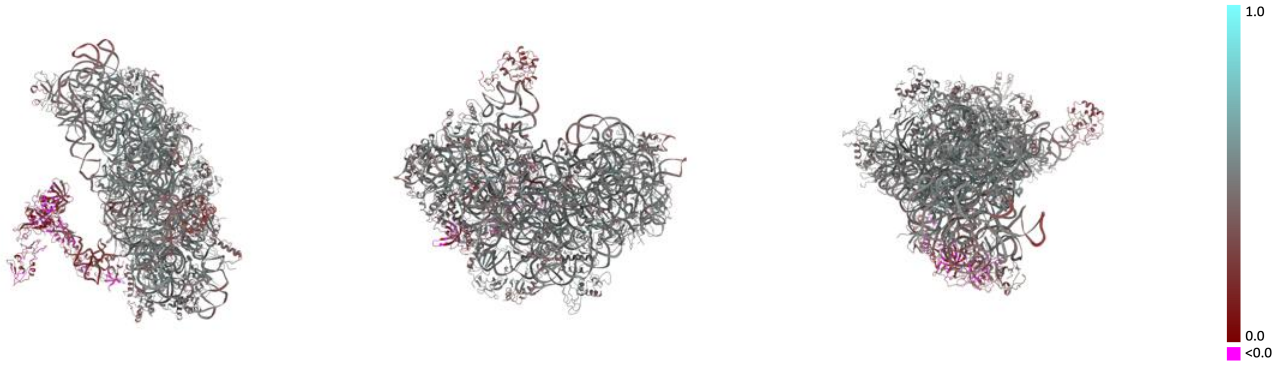
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.003 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.

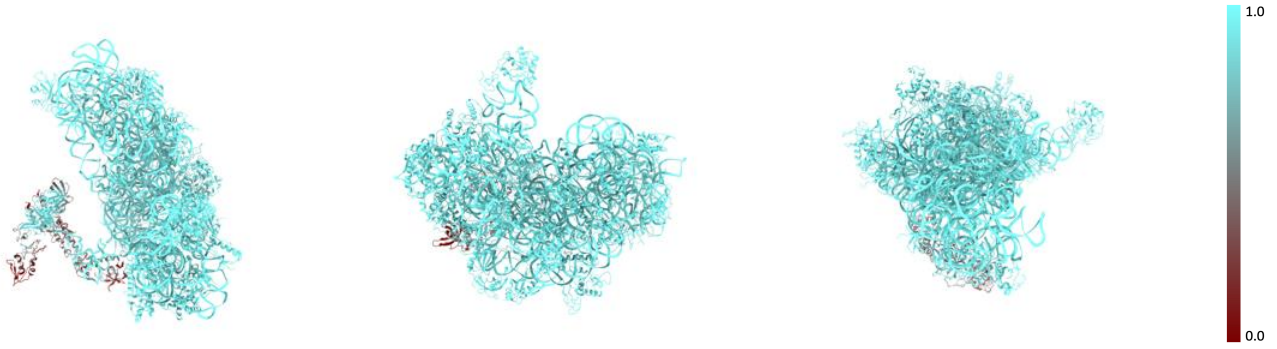
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according 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.

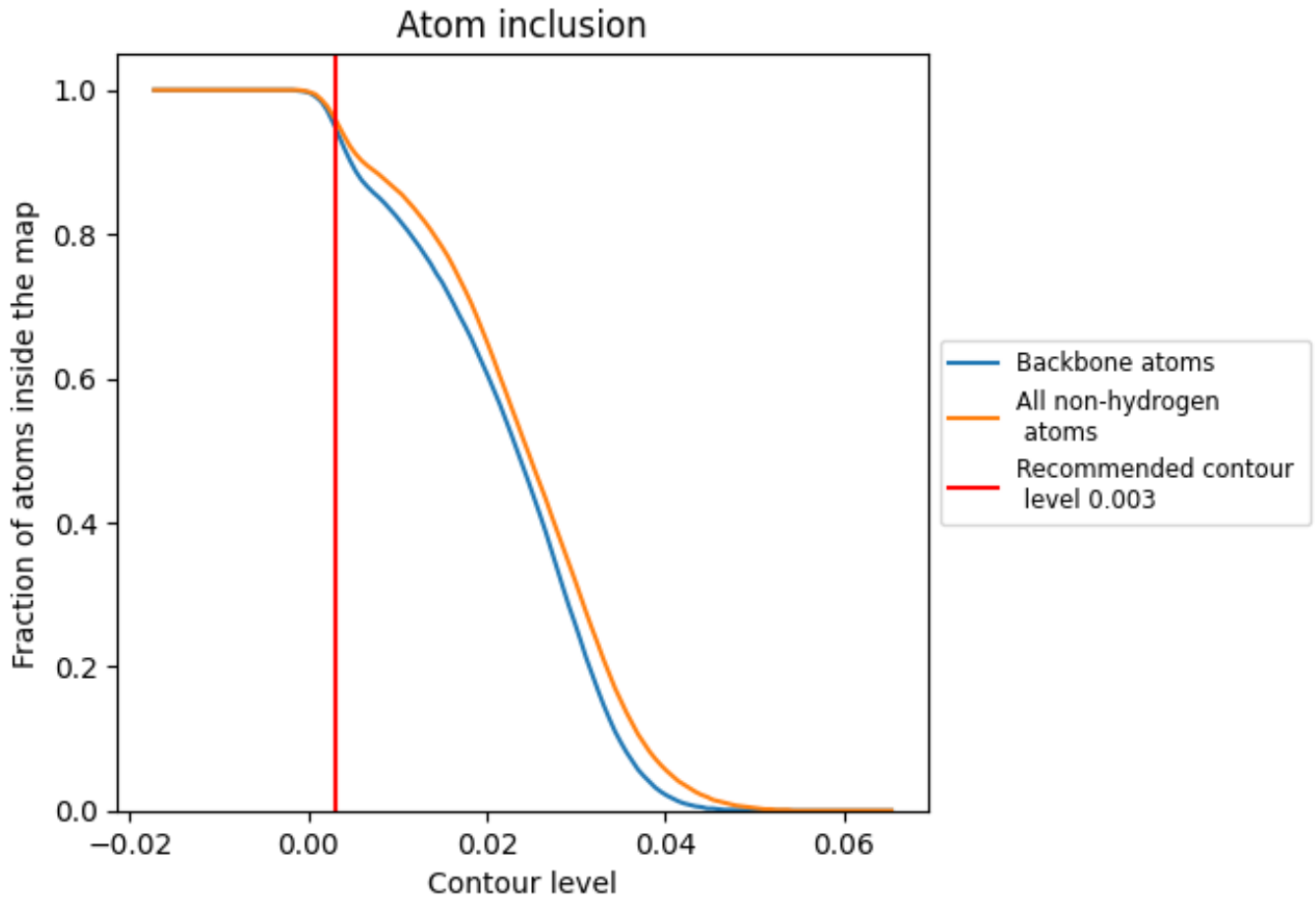
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.003).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.003) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9600	0.4380
0	1.0000	0.5010
2	1.0000	0.4860
3	0.9990	0.2680
4	0.9800	0.2700
5	1.0000	0.4290
6	0.9400	0.2860
7	0.7680	0.1590
8	0.3120	0.1710
9	0.3800	0.1540
A	0.9990	0.4620
B	0.9990	0.4620
C	0.9980	0.4570
D	0.9990	0.4770
E	1.0000	0.4840
F	0.9970	0.4830
G	1.0000	0.4200
H	0.9990	0.4660
I	0.9970	0.4910
J	1.0000	0.4780
K	0.9980	0.4850
L	0.9990	0.4530
M	1.0000	0.4840
N	1.0000	0.4820
O	1.0000	0.4500
P	1.0000	0.4910
Q	0.9990	0.4660
R	0.9980	0.4900
S	0.9910	0.4300
T	0.9990	0.4600
U	0.9950	0.4730
V	1.0000	0.4570
W	1.0000	0.4700
X	0.9980	0.4620
Y	1.0000	0.2540
Z	0.9980	0.4460