



Full wwPDB EM Validation Report ⓘ

Jun 22, 2026 – 11:08 PM EDT

PDB ID : 4V6V / pdb_00004v6v
EMDB ID : EMD-5562
Title : Tetracycline resistance protein Tet(O) bound to the ribosome
Authors : Li, W.; Atkinson, G.C.; Thakor, N.S.; Allas, U.; Lu, C.; Chan, K.Y.; Tenson, T.; Schulten, K.; Wilson, K.S.; Hauryliuk, V.; Frank, J.
Deposited on : 2013-02-25
Resolution : 9.80 Å(reported)
Based on initial models : 2I2U, 2I2V

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

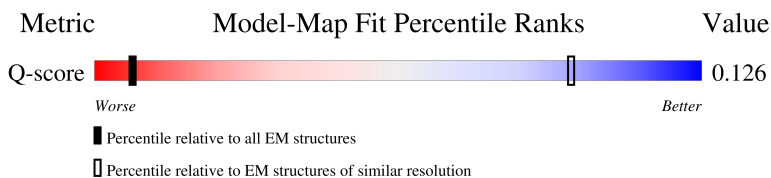
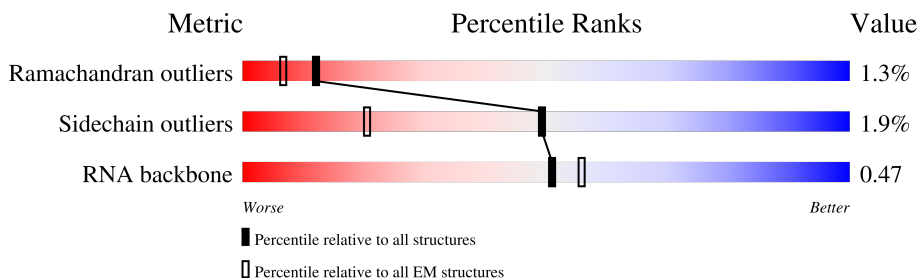
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance

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

The reported resolution of this entry is 9.80 Å.

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



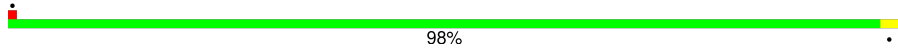
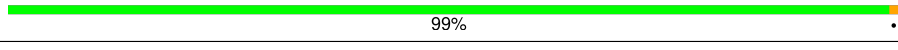
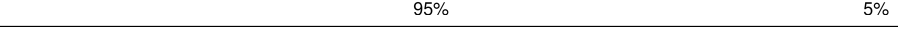
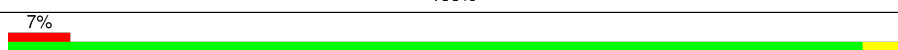
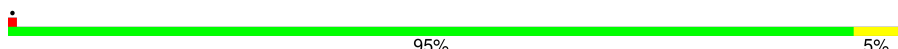
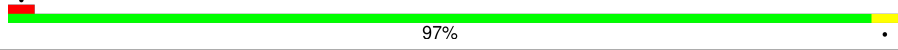
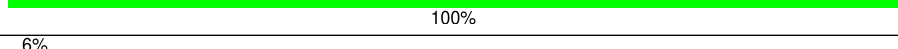
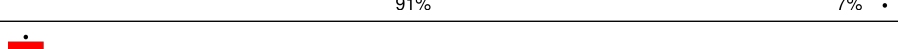
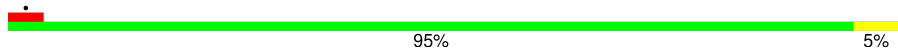
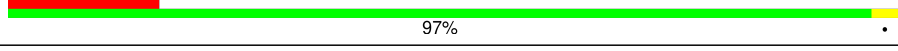
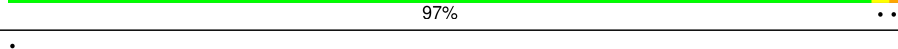
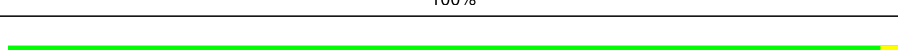
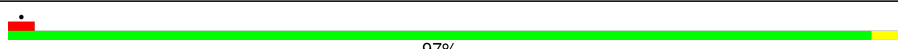
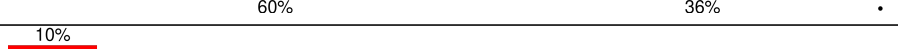
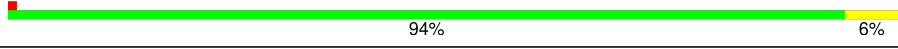
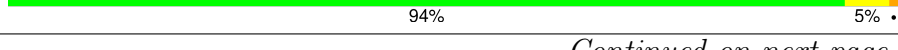
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	157 (9.30 - 10.30)

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

Mol	Chain	Length	Quality of chain
1	AJ	103	
2	AK	128	
3	AL	123	
4	AM	117	

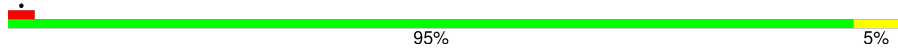
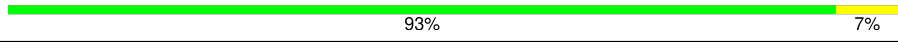
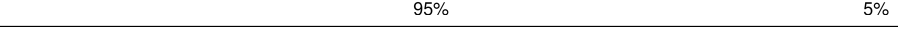
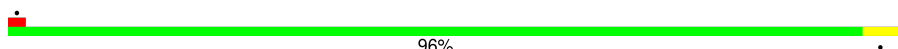
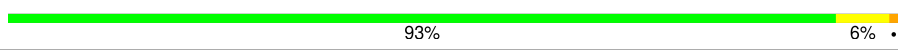
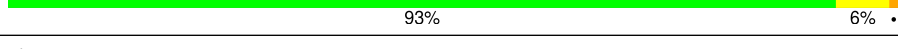
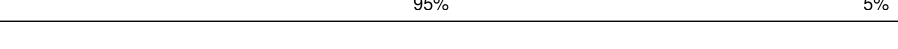
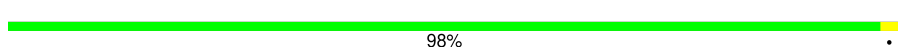
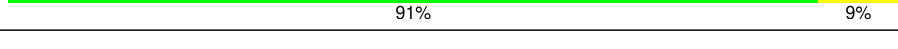
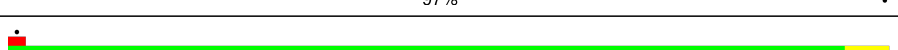
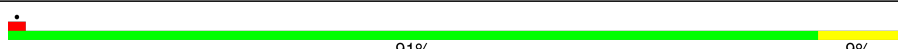
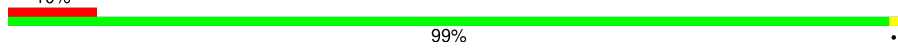
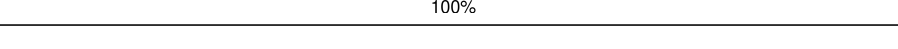
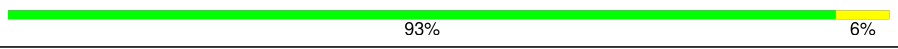
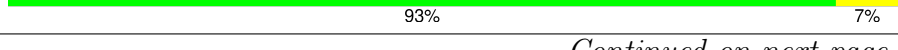
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Mol	Chain	Length	Quality of chain
5	AN	100	
6	AO	88	
7	AP	82	
8	AQ	83	
9	AR	74	
10	AS	91	
11	AB	240	
12	AT	86	
13	AU	70	
14	AC	232	
15	AD	205	
16	AE	166	
17	AF	135	
18	AG	178	
19	AH	129	
20	AI	129	
21	A1	639	
22	AA	1542	
23	A2	47	
24	A3	77	
25	BC	234	
26	BJ	164	
27	BK	141	
28	BN	142	
29	BO	123	

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Mol	Chain	Length	Quality of chain
30	BP	144	
31	BQ	136	
32	BR	127	
33	BS	117	
34	BT	114	
35	BD	272	
36	BU	117	
37	BV	103	
38	BW	110	
39	BX	100	
40	BY	103	
41	BZ	94	
42	B0	84	
43	B1	77	
44	B2	63	
45	BE	209	
46	B3	58	
47	B4	70	
48	B5	56	
49	B6	54	
50	B7	46	
51	B8	64	
52	B9	38	
53	BF	201	
54	BG	178	

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Mol	Chain	Length	Quality of chain
55	BH	176	 95% ..
56	BL	149	 18% 99% .
57	BA	2904	 63% 30% 6%
58	Ba	120	 77% 19% ..

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 154956 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AJ	103	Total	C	N	O	S	0	0
			794	483	158	151	2		

- Molecule 2 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AK	128	Total	C	N	O	S	0	0
			923	553	196	171	3		

- Molecule 3 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AL	123	Total	C	N	O	S	0	0
			923	558	196	165	4		

- Molecule 4 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AM	117	Total	C	N	O	S	0	0
			876	530	183	160	3		

- Molecule 5 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AN	100	Total	C	N	O	S	0	0
			771	465	164	139	3		

- Molecule 6 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AO	88	Total	C	N	O	S	0	0
			690	414	146	129	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AO	79	ARG	GLN	conflict	UNP P0ADZ4

- Molecule 7 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AP	82	Total	C	N	O	S	0	0
			620	377	128	114	1		

- Molecule 8 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AQ	83	Total	C	N	O	S	0	0
			657	410	124	120	3		

- Molecule 9 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AR	74	Total	C	N	O	S	0	0
			603	372	123	107	1		

- Molecule 10 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AS	91	Total	C	N	O	S	0	0
			708	445	139	122	2		

- Molecule 11 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AB	240	Total	C	N	O	S	0	0
			1805	1113	332	352	8		

- Molecule 12 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AT	86	Total	C	N	O	S	0	0
			636	380	138	115	3		

- Molecule 13 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AU	70	Total	C	N	O	S	0	0
			564	340	125	98	1		

- Molecule 14 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AC	232	Total	C	N	O	S	0	0
			1761	1088	346	323	4		

- Molecule 15 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AD	205	Total	C	N	O	S	0	0
			1587	970	315	298	4		

- Molecule 16 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AE	166	Total	C	N	O	S	0	0
			1182	718	232	226	6		

- Molecule 17 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AF	135	Total	C	N	O	S	0	0
			1061	637	198	219	7		

- Molecule 18 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AG	178	Total	C	N	O	S	0	0
			1347	821	269	253	4		

- Molecule 19 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AH	129	Total	C	N	O	S	0	0
			948	585	173	184	6		

- Molecule 20 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AI	129	Total	C	N	O	S	0	0
			1000	606	208	183	3		

- Molecule 21 is a protein called Tetracycline resistance protein TetO.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	A1	639	Total	C	N	O	S	0	0
			4989	3146	850	966	27		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A1	227	ILE	THR	conflict	UNP P10952

- Molecule 22 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AA	1542	Total	C	N	O	P	0	0
			33089	14767	6064	10717	1541		

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	A2	47	Total	C	N	O	P	0	0
			993	445	167	335	46		

- Molecule 24 is a RNA chain called P-tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	A3	77	Total	C	N	O	P	S	0	0
			1640	734	297	533	75	1		

- Molecule 25 is a protein called 50S ribosomal protein L1.

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

- Molecule 26 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BJ	164	Total	C	N	O	S	0	0
			1233	776	220	231	6		

- Molecule 27 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BK	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 28 is a protein called 50S ribosomal protein L13.

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

- Molecule 29 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BO	123	Total	C	N	O	S	0	0
			947	593	181	167	6		

- Molecule 30 is a protein called 50S ribosomal protein L15.

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

- Molecule 31 is a protein called 50S ribosomal protein L16.

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

- Molecule 32 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BR	127	Total	C	N	O	S	0	0
			1008	621	204	178	5		

- Molecule 33 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BS	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

- Molecule 34 is a protein called 50S ribosomal protein L19.

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

- Molecule 35 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BD	272	Total	C	N	O	S	0	0
			2092	1294	425	366	7		

- Molecule 36 is a protein called 50S ribosomal protein L20.

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

- Molecule 37 is a protein called 50S ribosomal protein L21.

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

- Molecule 38 is a protein called 50S ribosomal protein L22.

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

- Molecule 39 is a protein called 50S ribosomal protein L23.

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

- Molecule 40 is a protein called 50S ribosomal protein L24.

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

- Molecule 41 is a protein called 50S ribosomal protein L25.

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

- Molecule 42 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	B0	84	Total	C	N	O	S		
			634	391	129	113	1	0	0

- Molecule 43 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	B1	77	Total	C	N	O	S		
			625	388	129	106	2	0	0

- Molecule 44 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	B2	63	Total	C	N	O	S		
			509	313	99	95	2	0	0

- Molecule 45 is a protein called 50S ribosomal protein L3.

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

- Molecule 46 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	B3	58	Total	C	N	O	S		
			449	281	87	79	2	0	0

- Molecule 47 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	B4	70	Total	C	N	O	S	0	0
			549	339	104	100	6		

- Molecule 48 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	B5	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	B6	54	Total	C	N	O	S	0	0
			441	284	81	76			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	B7	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 51 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	B8	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 52 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	B9	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 53 is a protein called 50S ribosomal protein L4.

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

- Molecule 54 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BG	178	Total	C	N	O	S	0	0
			1420	905	251	258	6		

- Molecule 55 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BH	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 56 is a protein called 50S ribosomal protein L9.

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

- Molecule 57 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	BA	2904	Total	C	N	O	P	0	0
			62351	27824	11469	20155	2903		

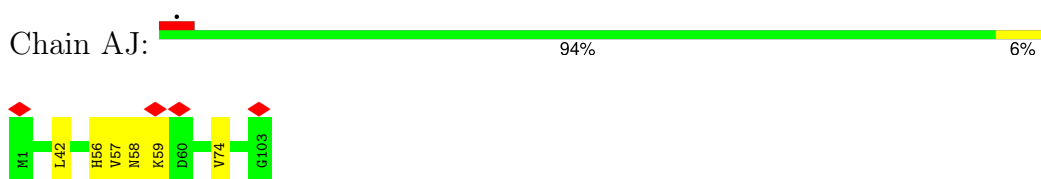
- Molecule 58 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Ba	120	Total	C	N	O	P	0	0
			2566	1144	468	835	119		

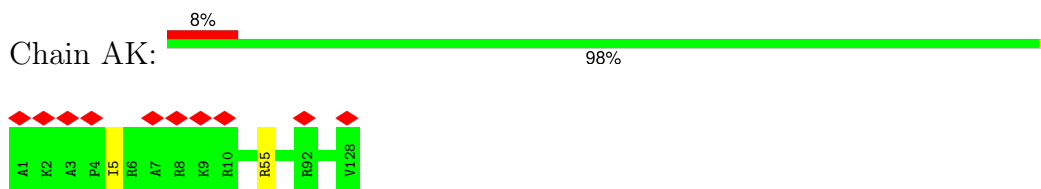
3 Residue-property plots [i](#)

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.

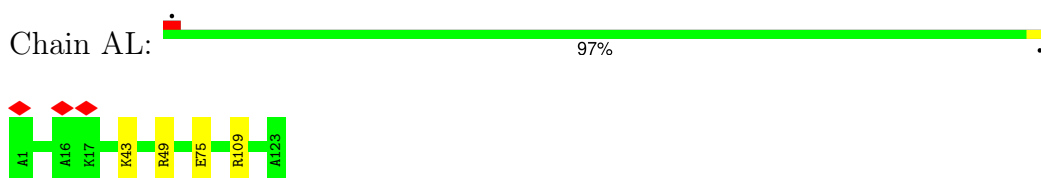
- Molecule 1: 30S ribosomal protein S10



- Molecule 2: 30S ribosomal protein S11



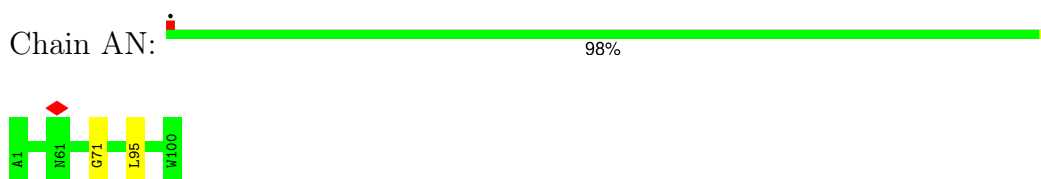
- Molecule 3: 30S ribosomal protein S12



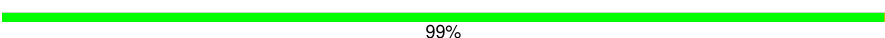
- Molecule 4: 30S ribosomal protein S13



- Molecule 5: 30S ribosomal protein S14

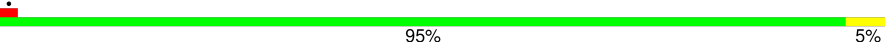


- Molecule 6: 30S ribosomal protein S15

Chain AO:  99%



- Molecule 7: 30S ribosomal protein S16

Chain AP:  95%

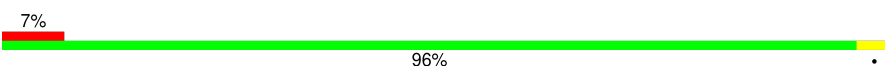


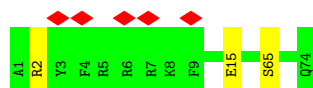
- Molecule 8: 30S ribosomal protein S17

Chain AQ:  100%

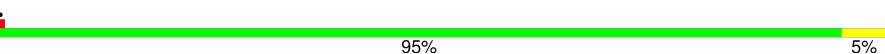
There are no outlier residues recorded for this chain.

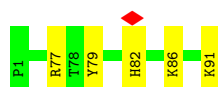
- Molecule 9: 30S ribosomal protein S18

Chain AR:  96%



- Molecule 10: 30S ribosomal protein S19

Chain AS:  95%

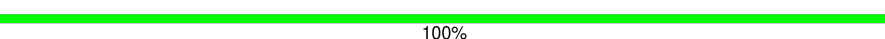


- Molecule 11: 30S ribosomal protein S2

Chain AB:  97%

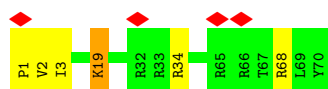
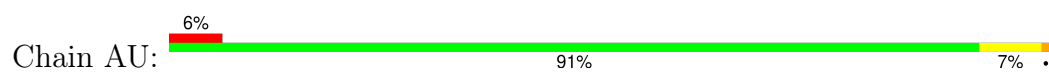


- Molecule 12: 30S ribosomal protein S20

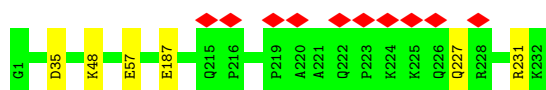
Chain AT:  100%

There are no outlier residues recorded for this chain.

- Molecule 13: 30S ribosomal protein S21



- Molecule 14: 30S ribosomal protein S3



- Molecule 15: 30S ribosomal protein S4



- Molecule 16: 30S ribosomal protein S5



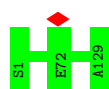
- Molecule 17: 30S ribosomal protein S6



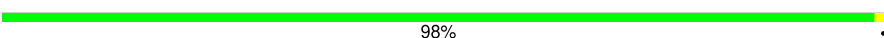
- Molecule 18: 30S ribosomal protein S7



- Molecule 19: 30S ribosomal protein S8

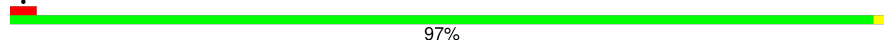


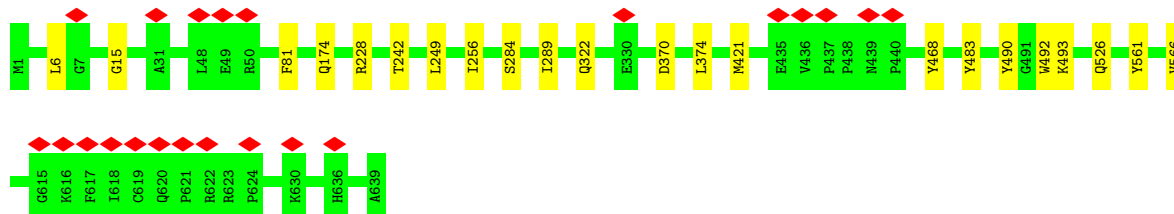
- Molecule 20: 30S ribosomal protein S9

Chain AI:  98%



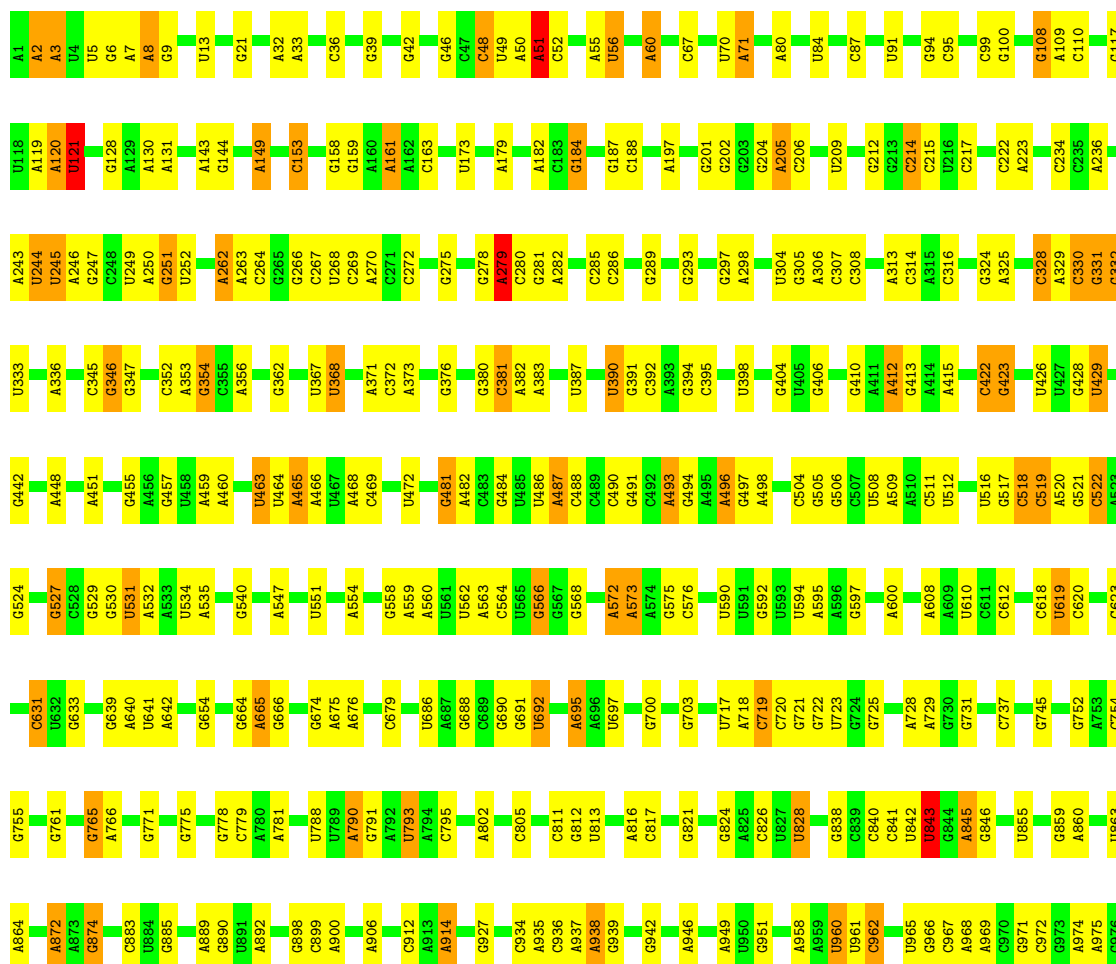
- Molecule 21: Tetracycline resistance protein TetO

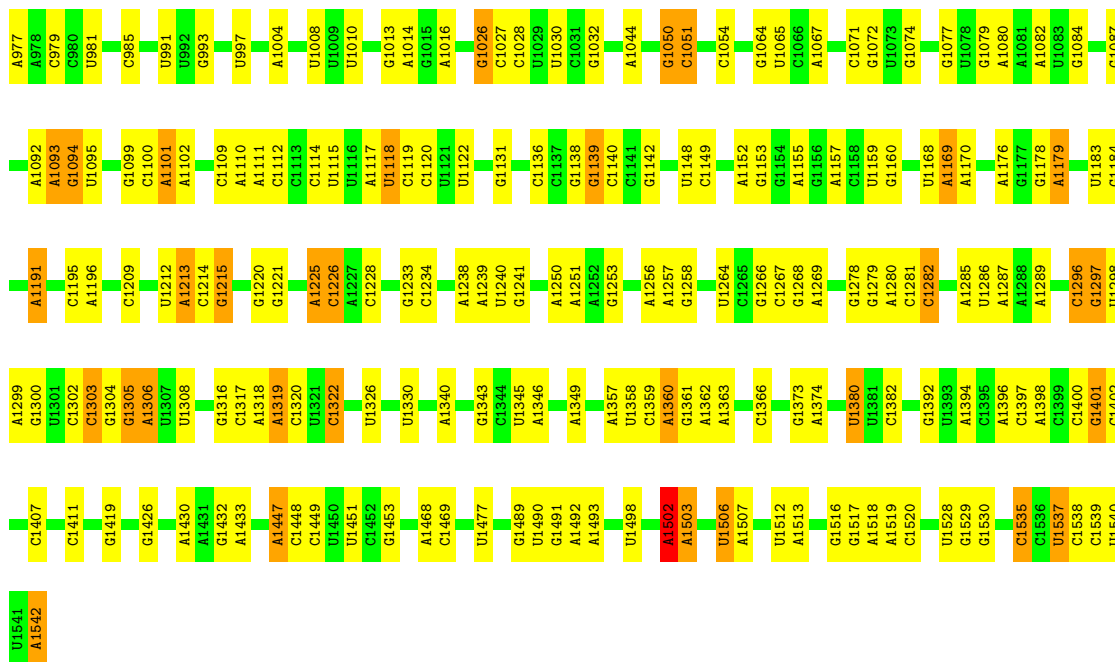
Chain A1:  97%



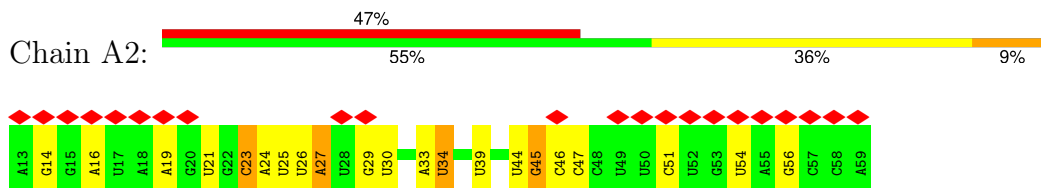
- Molecule 22: 16S ribosomal RNA

Chain AA:  65% 29% 6%

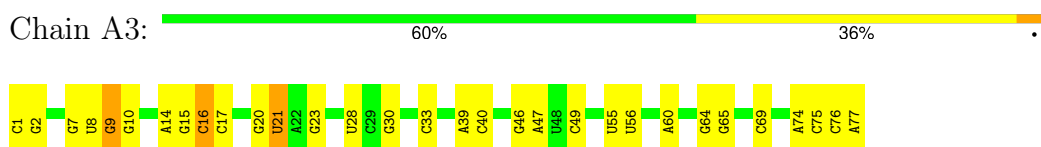




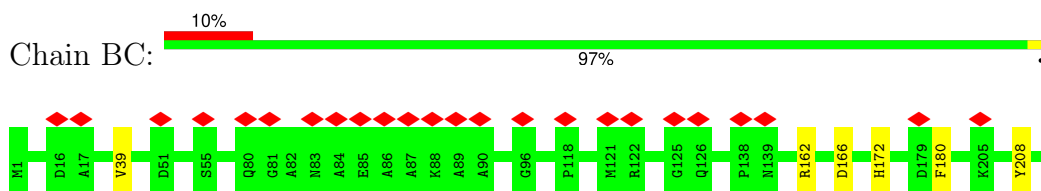
- Molecule 23: mRNA



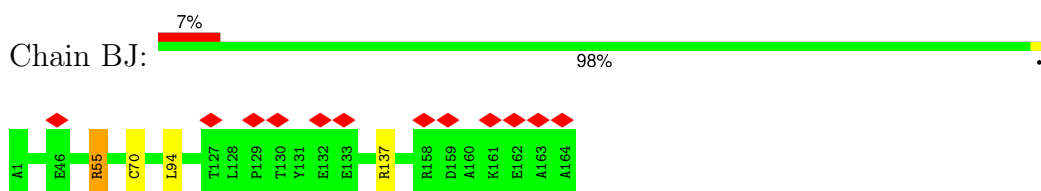
- Molecule 24: P-tRNA



- Molecule 25: 50S ribosomal protein L1

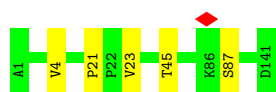


- Molecule 26: 50S ribosomal protein L10



- Molecule 27: 50S ribosomal protein L11

Chain BK:  96% .



- Molecule 28: 50S ribosomal protein L13

Chain BN:  94% 6% .



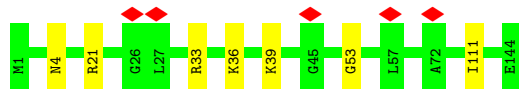
- Molecule 29: 50S ribosomal protein L14

Chain BO:  94% 5% .



- Molecule 30: 50S ribosomal protein L15

Chain BP:  95% 5% .

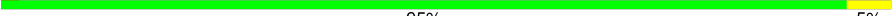


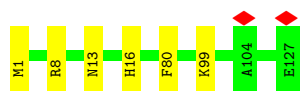
- Molecule 31: 50S ribosomal protein L16

Chain BQ:  93% 7% .



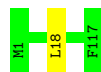
- Molecule 32: 50S ribosomal protein L17

Chain BR:  95% 5% .

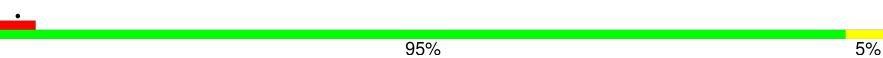


- Molecule 33: 50S ribosomal protein L18

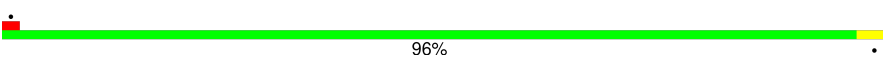
Chain BS:  99% .



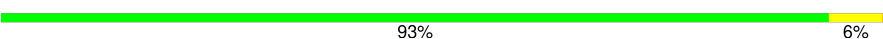
• Molecule 34: 50S ribosomal protein L19

Chain BT:  95% 5%

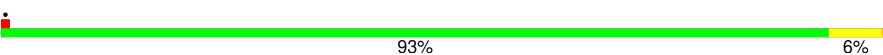
• Molecule 35: 50S ribosomal protein L2

Chain BD:  96%

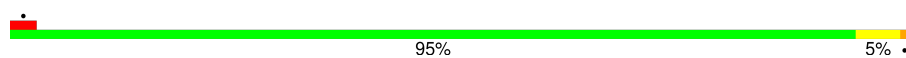
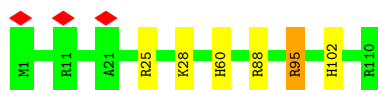
• Molecule 36: 50S ribosomal protein L20

Chain BU:  93% 6%

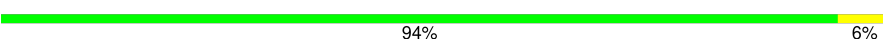
• Molecule 37: 50S ribosomal protein L21

Chain BV:  93% 6%

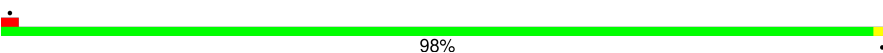
• Molecule 38: 50S ribosomal protein L22

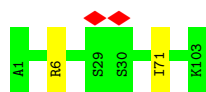
Chain BW:  95% 5%

• Molecule 39: 50S ribosomal protein L23

Chain BX:  94% 6%

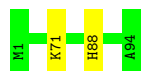
• Molecule 40: 50S ribosomal protein L24

Chain BY:  98%



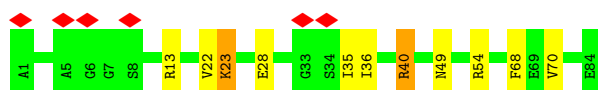
- Molecule 41: 50S ribosomal protein L25

Chain BZ: 98%



- Molecule 42: 50S ribosomal protein L27

Chain B0: 7% 87% 11%



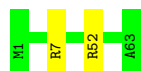
- Molecule 43: 50S ribosomal protein L28

Chain B1: 91% 9%



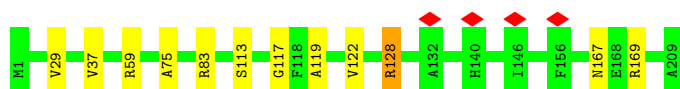
- Molecule 44: 50S ribosomal protein L29

Chain B2: 97%



- Molecule 45: 50S ribosomal protein L3

Chain BE: 94% 5%

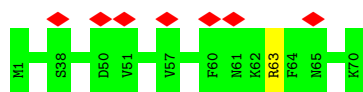


- Molecule 46: 50S ribosomal protein L30

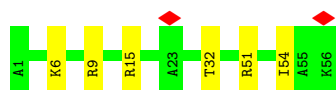
Chain B3: 91% 9%



- Molecule 47: 50S ribosomal protein L31



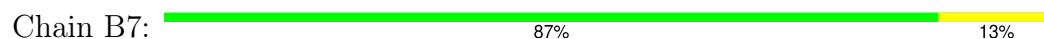
- Molecule 48: 50S ribosomal protein L32



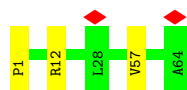
- Molecule 49: 50S ribosomal protein L33



- Molecule 50: 50S ribosomal protein L34



- Molecule 51: 50S ribosomal protein L35



- Molecule 52: 50S ribosomal protein L36



- Molecule 53: 50S ribosomal protein L4

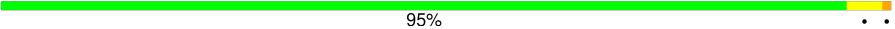


- Molecule 54: 50S ribosomal protein L5

Chain BG:  93% 7%

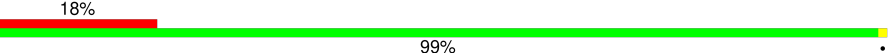


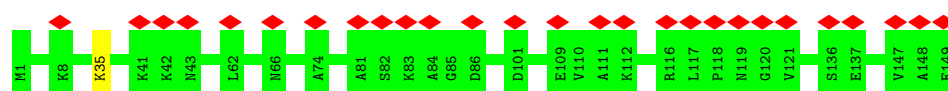
- Molecule 55: 50S ribosomal protein L6

Chain BH:  95%



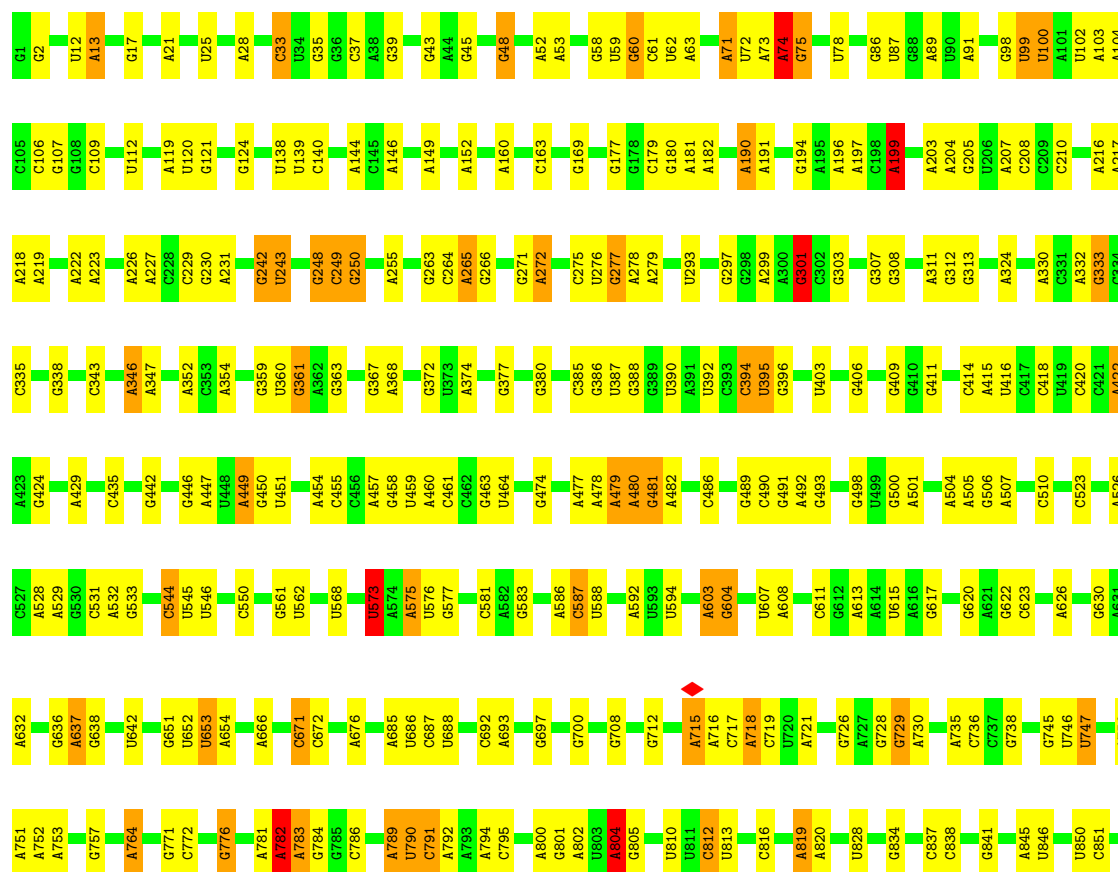
- Molecule 56: 50S ribosomal protein L9

Chain BL:  18% 99%

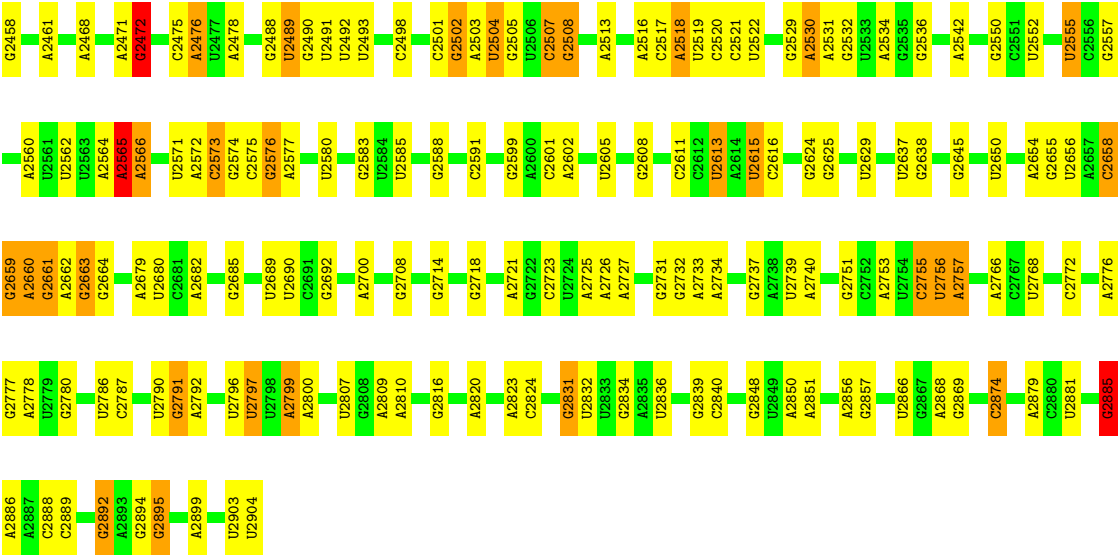


- Molecule 57: 23S ribosomal RNA

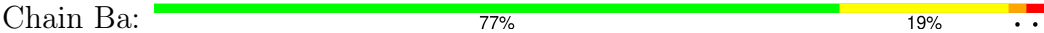
Chain BA:  63% 30% 6%



A2369	A2375	A2376	G2382	G2383	G2384	G2385	G2390	G2391	A2392	G2399	G2400	G2401	G2402	G2403	G2404	G2405	G2408	A2411	G2420	G2421	G2422	G2423	G2424	G2425	G2426	G2427	G2428	G2429	G2430	G2431	G2432	G2433	G2434	G2435	G2436	G2437	G2438	G2439	G2440	G2441	G2442	G2447	G2448	G2449	G2450	G2451	G2452	G2453	G2457																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
C2254	C2258	C2261	A2266	A2267	A2268	A2273	A2274	G2275	G2276	G2282	G2283	A2284	G2286	A2287	G2288	G2289	C2295	C2300	C2301	G2304	G2305	G2306	G2307	G2308	A2309	G2312	G2321	G2322	G2323	G2324	G2325	G2326	A2327	A2333	A2334	A2335	A2336	A2337	G2341	G2345	A2346	G2347	A2451	G2357	A2358	G2359	G2365																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
G2138	C2146	A2147	G2148	G2152	C2153	A2154	A2158	C2164	C2165	G2166	G2167	G2168	A2169	A2170	G2182	G2188	G2197	A2198	A2199	G2202	G2203	G2204	G2205	G2206	G2210	G2211	G2212	G2213	G2226	G2227	G2228	G2229	G2230	G2236	G2239	G2243	G2244	G2245	G2246	A2247	G2248	G2249	G2250	G2251	G2252	G2253																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
A2042	C2043	C2050	A2051	G2052	G2053	A2054	G2055	G2056	G2057	G2058	A2059	A2060	G2061	A2062	G2063	C2064	C2065	G2068	G2069	G2074	G2075	A2076	A2077	A2080	A2080	C2091	G2092	G2093	A2097	G2102	G2111	G2112	G2113	G2114	G2115	G2116	A2117	G2118	A2119	G2120	A2126	G2127	G2130	G2131	G2132	A2134	G2135																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
A1928	G1929	G1930	A1937	A1938	G1939	G1940	C1942	G1943	G1944	G1945	G1948	A1953	A1954	G1955	G1962	G1963	G1964	A1965	A1966	A1970	G1971	G1972	G1973	G1976	G1982	G1992	G1993	C1996	C1997	A1998	G2002	G2007	G2011	G2012	A2019	G2023	A2030	A2031	G2032	A2033	G2034	G2035																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
A1828	G1829	A1830	A1831	G1832	G1833	G1834	G1835	G1836	G1837	G1838	G1839	G1842	A1848	G1851	G1857	G1864	G1865	G1866	G1869	G1870	G1881	G1882	G1883	G1884	A1885	A1900	A1901	G1906	G1911	A1912	A1913	G1914	G1915	G1916	G1917	A1918	A1919	G1922	G1926	G1927	G1928	G1929	G1930	G1931	G1932	G1933	G1934	G1935	G1936	G1937	G1938	G1939	G1940	G1941	G1942	G1943	G1944	G1945	G1946	G1947	G1948	G1949	G1950	G1951	G1952	G1953	G1954	G1955	G1956	G1957	G1958	G1959	G1960	G1961	G1962	G1963	G1964	G1965	G1966	G1967	G1968	G1969	G1970	G1971	G1972	G1973	G1974	G1975	G1976	G1977	G1978	G1979	G1980	G1981	G1982	G1983	G1984	G1985	G1986	G1987	G1988	G1989	G1990	G1991	G1992	G1993	G1994	G1995	G1996	G1997	G1998	G1999	G2000	G2001	G2002	G2003	G2004	G2005	G2006	G2007	G2008	G2009	G2010	G2011	G2012	G2013	G2014	G2015	G2016	G2017	G2018	G2019	G2020	G2021	G2022	G2023	G2024	G2025	G2026	G2027	G2028	G2029	G2030	G2031	G2032	G2033	G2034	G2035	G2036	G2037	G2038	G2039	G2040	G2041	G2042	G2043	G2044	G2045	G2046	G2047	G2048	G2049	G2050	G2051	G2052	G2053	G2054	G2055	G2056	G2057	G2058	G2059	G2060	G2061	G2062	G2063	G2064	G2065	G2066	G2067	G2068	G2069	G2070	G2071	G2072	G2073	G2074	G2075	G2076	G2077	G2078	G2079	G2080	G2081	G2082	G2083	G2084	G2085	G2086	G2087	G2088	G2089	G2090	G2091	G2092	G2093	G2094	G2095	G2096	G2097	G2098	G2099	G2100	G2101	G2102	G2103	G2104	G2105	G2106	G2107	G2108	G2109	G2110	G2111	G2112	G2113	G2114	G2115	G2116	G2117	G2118	G2119	G2120	G2121	G2122	G2123	G2124	G2125	G2126	G2127	G2128	G2129	G2130	G2131	G2132	G2133	G2134	G2135	G2136	G2137	G2138	G2139	G2140	G2141	G2142	G2143	G2144	G2145	G2146	G2147	G2148	G2149	G2150	G2151	G2152	G2153	G2154	G2155	G2156	G2157	G2158	G2159	G2160	G2161	G2162	G2163	G2164	G2165	G2166	G2167	G2168	G2169	G2170	G2171	G2172	G2173	G2174	G2175	G2176	G2177	G2178	G2179	G2180	G2181	G2182	G2183	G2184	G2185	G2186	G2187	G2188	G2189	G2190	G2191	G2192	G2193	G2194	G2195	G2196	G2197	G2198	G2199	G2200	G2201	G2202	G2203	G2204	G2205	G2206	G2207	G2208	G2209	G2210	G2211	G2212	G2213	G2214	G2215	G2216	G2217	G2218	G2219	G2220	G2221	G2222	G2223	G2224	G2225	G2226	G2227	G2228	G2229	G2230	G2231	G2232	G2233	G2234	G2235	G2236	G2237	G2238	G2239	G2240	G2241	G2242	G2243	G2244	G2245	G2246	G2247	G2248	G2249	G2250	G2251	G2252	G2253	G2254	G2255	G2256	G2257	G2258	G2259	G2260	G2261	G2262	G2263	G2264	G2265	G2266	G2267	G2268	G2269	G2270	G2271	G2272	G2273	G2274	G2275	G2276	G2277	G2278	G2279	G2280	G2281	G2282	G2283	G2284	G2285	G2286	G2287	G2288	G2289	G2290	G2291	G2292	G2293	G2294	G2295	G2296	G2297	G2298	G2299	G2300	G2301	G2302	G2303	G2304	G2305	G2306	G2307	G2308	G2309	G2310	G2311	G2312	G2313	G2314	G2315	G2316	G2317	G2318	G2319	G2320	G2321	G2322	G2323	G2324	G2325	G2326	G2327	G2328	G2329	G2330	G2331	G2332	G2333	G2334	G2335	G2336	G2337	G2338	G2339	G2340	G2341	G2342	G2343	G2344	G2345	G2346	G2347	G2348	G2349	G2350	G2351	G2352	G2353	G2354	G2355	G2356	G2357	G2358	G2359	G2360	G2361	G2362	G2363	G2364	G2365	G2366	G2367	G2368	G2369	G2370	G2371	G2372	G2373	G2374	G2375	G2376	G2377	G2378	G2379	G2380	G2381	G2382	G2383	G2384	G2385	G2386	G2387	G2388	G2389	G2390	G2391	G2392	G2393	G2394	G2395	G2396	G2397	G2398	G2399	G2400	G2401	G2402	G2403	G2404	G2405	G2406	G2407	G2408	G2409	G2410	G2411	G2412	G2413	G2414	G2415	G2416	G2417	G2418	G2419	G2420	G2421	G2422	G2423	G2424	G2425	G2426	G2427	G2428	G2429	G2430	G2431	G2432	G2433	G2434	G2435	G2436	G2437	G2438	G2439	G2440	G2441	G2442	G2443	G2444	G2445	G2446	G2447	G2448	G2449	G2450	G2451	G2452	G2453	G2454	G2455	G2456	G2457	G2458	G2459	G2460	G2461	G2462	G2463	G2464	G2465	G2466	G2467	G2468	G2469	G2470	G2471	G2472	G2473	G2474	G2475	G2476	G2477	G2478	G2479	G2480	G2481	G2482	G2483	G2484	G2485	G2486	G2487	G2488	G2489	G2490	G2491	G2492	G2493	G2494	G2495	G2496	G2497	G2498	G2499	G2500	G2501	G2502	G2503	G2504	G2505	G2506	G2507	G2508	G2509	G2510	G2511	G2512	G2513	G2514	G2515	G2516	G2517	G2518	G2519	G2520	G2521	G2522	G2523	G2524	G2525	G2526	G2527	G2528	G2529	G2530	G2531	G2532	G2533	G2534	G2535	G2536	G2537	G2538	G2539	G2540	G2541	G2542	G2543	G2544	G2545	G2546	G2547	G2548	G2549	G2550	G2551	G2552	G2553	G2554	G2555	G2556	G2557	G2558	G2559	G2560	G2561	G2562	G2563	G2564	G2565	G2566	G2567	G2568	G2569	G2570	G2571	G2572	G2573	G2574	G2575	G2576	G2577	G2578	G2579	G2580	G2581	G2582	G2583	G2584	G2585	G2586	G2587	G2588	G2589	G2590	G2591	G2592	G2593	G2594	G2595	G2596	G2597	G2598	G2599	G2600	G2601	G2602	G2603	G2604	G2605	G2606	G2607	G2608	G2609	G2610	G2611	G2612	G2613	G2614	G2615	G2616	G2617	G2618	G2619	G2620	G2621	G2622	G2623	G2624	G2625	G2626	G2627	G2628	G2629	G2630	G2631	G2632	G2633	G2634	G2635	G2636	G2637	G2638	G2639	G2640	G2641	G2642	G2643	G2644	G2645	G2646	G2647	G2648	G2649	G2650	G2651	G2652	G2653	G2654	G2655	G2656	G2657	G2658	G2659	G2660	G2661	G2662	G2663	G2664	G2665	G2666	G2667	G2668	G2669	G2670	G2671	G2672	G2673	G2674	G2675	G2676	G2677	G2678	G2679	G2680	G2681	G2682	G2683	G2684	G2685	G2686	G2687	G2688	G2689	G2690	G2691	G2692	G2693	G2694	G2695	G2696	G2697	G2698	G2699	G2700	G2701	G2702	G2703	G2704	G2705	G2706	G2707	G2708	G2709	G2710	G2711	G2712	G2713	G2714	G2715	G2716	G2717	G2718	G2719	G2720	G2721	G2722	G2723	G2724	G2725	G2726	G2727	G2728	G2729	G2730	G2731	G2732	G2733	G2734	G2735	G2736	G2737	G2738	G2739	G2740	G2741	G2742	G2743	G2744	G2745	G2746	G2747	G2748	G2749	G2750	G2751	G2752	G2753	G2754	G2755	G2756	G2757	G2758	G2759	G2760	G2761	G2762	G2763	G2764	G2765	G2766	G2767	G2768	G2769	G2770	G2771	G2772	G2773	G2774	G2775	G2776	G2777	G2778	G2779	G2780	G2781	G2782	G2783	G2784	G2785	G2786	G2787	G2788	G2789	G2790	G2791	G2792	G2793	G2794	G2795	G2796	G2797	G2798	G2799	G2800	G2801	G2802	G2803	G2804	G2805	G2806	G2807	G2808	G2809	G2810	G2811	G2812	G2813	G2814	G2815	G2816	G2817	G2818	G2819	G2820	G2821	G2822	G2823	G2824	G2825	G2826	G2827	G2828	G2829	G2830	G2831	G2832	G2833	G2834	G2835	G2836	G2837	G2838	G2839	G2840	G2841	G2842	G2843	G2844	G2845	G2846	G2847	G2848	G2849	G2850	G2851	G2852	G2853	G2854	G2855	G2856	G2857	G2858	G2859	G2860	G2861	G2862	G2863	G2864	G2865	G2866	G2867	G2868	G2869	G2870	G2871	G2872	G2873	G2874	G2875	G2876	G2877	G2878	G2879	G2880	G2881	G2882	G2883	G2884	G2885	G2886	G2887	G2888	G2889	G2890	G2891	G2892	G2893	G2894	G2895	G2896	G2897	G2898	G2899	G2900	G2901	G2902	G2903	G2904	G2905	G2906	G2907	G2908	G2909	G2910	G2911	G2912	G2913	G2914	G2915	G2916	G2917	G2918	G2919	G2920	G2921	G2922	G2923	G2924	G2925	G2926	G2927	G2928	G2929	G2930	G2931	G2932	G2933	G2934	G2935	G2936	G2937	G2938	G2939	G2940	G2941	G2942	G2943	G2944	G2945	G2946	G2947	G2948	G2949	G2950	G2951	G2952	G2953	G2954	G2955	G2956	G2957	G2958	G2959	G2960	G2961	G2962	G2963	G2964	G2965	G2966	G2967	G2968	G2969	G2970	G2971	G2972	G2973	G2974	G2975	G2976	G2977	G2978	G2979	G2980	G2981	G2982	G2983	G2984	G2985	G2986	G2987	G2988	G2989	G2990	G2991	G2992	G2993	G2994	G2995	G2996	G2997	G2998	G2999	G3000	G3001	G3002	G3003	G3004	G3005	G3006	G3007	G3008	G30



● Molecule 58: 5S ribosomal RNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	98000	Depositor
Resolution determination method	FSC	Depositor
CTF correction method	group defocus	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	10	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	Not provided	
Maximum map value	253.190	Depositor
Minimum map value	-113.794	Depositor
Average map value	4.829	Depositor
Map value standard deviation	25.951	Depositor
Recommended contour level	22	Depositor
Map size ($\text{\AA}$)	365.85, 365.85, 365.85	wwPDB
Map dimensions	135, 135, 135	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	2.71, 2.71, 2.71	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	AJ	0.86	0/742	1.35	2/941 (0.2%)
2	AK	0.88	0/856	1.39	0/1069
3	AL	0.88	0/873	1.35	0/1110
4	AM	0.89	0/817	1.36	0/1022
5	AN	0.89	0/715	1.33	0/883
6	AO	0.86	0/646	1.31	0/813
7	AP	0.87	0/572	1.35	2/711 (0.3%)
8	AQ	0.83	0/636	1.31	0/822
9	AR	0.95	0/568	1.34	0/713
10	AS	0.91	0/687	1.35	1/880 (0.1%)
11	AB	0.82	0/1703	1.28	4/2161 (0.2%)
12	AT	0.85	0/574	1.33	0/694
13	AU	0.96	0/520	1.40	3/636 (0.5%)
14	AC	0.83	0/1669	1.25	1/2122 (0.0%)
15	AD	0.85	0/1497	1.30	1/1890 (0.1%)
16	AE	0.85	0/1110	1.34	3/1405 (0.2%)
17	AF	0.86	0/1001	1.31	0/1268
18	AG	0.83	0/1263	1.30	2/1590 (0.1%)
19	AH	0.79	0/896	1.28	0/1141
20	AI	0.89	0/940	1.35	2/1180 (0.2%)
21	A1	0.86	0/4864	1.38	9/6363 (0.1%)
22	AA	0.85	1/36769 (0.0%)	1.19	70/57354 (0.1%)
23	A2	0.91	0/1108	1.24	8/1724 (0.5%)
24	A3	0.88	1/1717 (0.1%)	1.17	2/2675 (0.1%)
25	BC	0.90	0/1748	1.39	2/2355 (0.1%)
26	BJ	0.89	0/1247	1.40	1/1679 (0.1%)
27	BK	0.88	0/1046	1.44	3/1410 (0.2%)
28	BN	0.96	0/1152	1.44	3/1551 (0.2%)
29	BO	0.95	0/956	1.39	1/1279 (0.1%)
30	BP	0.98	0/1062	1.48	1/1413 (0.1%)
31	BQ	0.95	1/1093 (0.1%)	1.47	4/1460 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	BR	0.96	0/1021	1.48	0/1364
33	BS	0.91	0/910	1.38	0/1219
34	BT	0.94	0/929	1.41	2/1242 (0.2%)
35	BD	0.97	0/2131	1.45	4/2863 (0.1%)
36	BU	0.90	0/960	1.49	2/1278 (0.2%)
37	BV	0.90	0/829	1.39	4/1107 (0.4%)
38	BW	0.88	0/864	1.36	3/1156 (0.3%)
39	BX	0.88	0/794	1.41	2/1060 (0.2%)
40	BY	0.88	0/797	1.36	0/1062
41	BZ	0.87	0/766	1.36	1/1025 (0.1%)
42	B0	1.00	0/642	1.53	3/848 (0.4%)
43	B1	0.97	0/635	1.48	6/848 (0.7%)
44	B2	0.87	0/510	1.48	2/677 (0.3%)
45	BE	0.91	0/1586	1.49	6/2134 (0.3%)
46	B3	0.95	0/453	1.48	7/605 (1.2%)
47	B4	1.02	0/559	1.44	0/745
48	B5	1.02	0/450	1.54	3/599 (0.5%)
49	B6	0.87	0/448	1.32	0/594
50	B7	1.04	0/380	1.60	6/498 (1.2%)
51	B8	1.02	0/513	1.49	1/676 (0.1%)
52	B9	0.93	0/303	1.37	0/397
53	BF	0.89	0/1571	1.44	10/2113 (0.5%)
54	BG	0.91	0/1444	1.40	5/1937 (0.3%)
55	BH	0.92	0/1343	1.44	1/1816 (0.1%)
56	BL	0.91	0/1122	1.39	0/1515
57	BA	0.85	1/69280 (0.0%)	1.20	135/108078 (0.1%)
58	Ba	0.85	0/2869	1.17	7/4474 (0.2%)
All	All	0.87	4/165156 (0.0%)	1.26	335/244244 (0.1%)

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
3	AL	0	1
6	AO	0	1
7	AP	0	1
9	AR	0	1
10	AS	0	1
15	AD	0	1
18	AG	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
21	A1	0	2
22	AA	0	350
23	A2	0	5
24	A3	0	15
26	BJ	0	1
28	BN	0	2
29	BO	0	1
32	BR	0	1
34	BT	0	1
35	BD	0	1
36	BU	0	2
38	BW	0	1
40	BY	0	1
42	B0	0	1
51	B8	0	1
55	BH	0	2
57	BA	0	660
58	Ba	0	15
All	All	0	1070

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	AA	1498	UR3	O3'-P	6.64	1.62	1.56
57	BA	2552	OMU	O3'-P	6.55	1.62	1.56
24	A3	8	4SU	O3'-P	5.43	1.61	1.56
31	BQ	81	ARG	CZ-NH2	-5.06	1.26	1.33

All (335) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	2061	G	C2'-C3'-O3'	8.75	122.63	109.50
22	AA	1118	U	C5'-C4'-C3'	-8.37	103.45	116.00
57	BA	2658	C	C4'-C3'-C2'	-8.09	94.51	102.60
57	BA	2661	G	C1'-O4'-C4'	-8.02	101.89	109.90
48	B5	9	ARG	NE-CZ-NH2	7.62	126.06	119.20
23	A2	24	A	O3'-P-O5'	-7.22	93.16	104.00
36	BU	5	ARG	NE-CZ-NH2	7.12	125.61	119.20
57	BA	2199	A	C5'-C4'-C3'	-7.12	105.32	116.00
22	AA	328	C	C2'-C3'-O3'	7.11	120.17	109.50
57	BA	1332	G	C4'-C3'-O3'	7.07	120.00	109.40
11	AB	49	PHE	CA-CB-CG	7.06	120.86	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	60	G	O3'-P-O5'	-7.04	93.44	104.00
53	BF	130	LYS	CA-C-N	6.96	129.49	120.44
53	BF	130	LYS	C-N-CA	6.96	129.49	120.44
11	AB	68	PHE	CA-CB-CG	6.83	120.63	113.80
51	B8	1	PRO	CA-N-CD	-6.81	102.46	112.00
21	A1	15	GLY	CA-C-N	6.75	129.65	120.54
21	A1	15	GLY	C-N-CA	6.75	129.65	120.54
22	AA	463	U	O4'-C4'-C3'	6.72	110.72	104.00
16	AE	111	ARG	NH1-CZ-NH2	-6.71	110.58	119.30
37	BV	68	ARG	NE-CZ-NH2	6.68	125.21	119.20
57	BA	346	A	O4'-C1'-N9	6.67	118.50	108.50
18	AG	1	PRO	CA-N-CD	-6.64	102.71	112.00
22	AA	275	G	C5'-C4'-C3'	-6.58	106.13	116.00
58	Ba	10	G	C5'-C4'-C3'	-6.57	106.14	116.00
57	BA	2791	G	C2'-C3'-O3'	6.56	119.34	109.50
34	BT	38	ARG	NE-CZ-NH2	6.54	125.09	119.20
7	AP	32	PHE	CA-CB-CG	6.48	120.28	113.80
38	BW	95	ARG	NE-CZ-NH2	6.47	125.03	119.20
57	BA	199	A	O3'-P-O5'	-6.44	94.34	104.00
16	AE	111	ARG	NE-CZ-NH1	6.43	127.93	121.50
37	BV	84	ARG	NE-CZ-NH2	6.43	124.99	119.20
57	BA	1772	A	C4'-C3'-C2'	-6.43	96.17	102.60
21	A1	81	PHE	CA-CB-CG	6.42	120.22	113.80
57	BA	99	U	O4'-C1'-N1	6.41	117.81	108.20
22	AA	519	C	C5'-C4'-C3'	-6.40	105.60	115.20
54	BG	106	ALA	CA-C-N	6.40	124.27	120.24
54	BG	106	ALA	C-N-CA	6.40	124.27	120.24
57	BA	479	A	C2'-C3'-O3'	6.39	119.08	109.50
22	AA	793	U	O4'-C1'-N1	6.29	117.93	108.50
13	AU	1	PRO	CA-N-CD	-6.29	103.20	112.00
21	A1	6	LEU	CA-C-N	6.28	125.92	121.65
21	A1	6	LEU	C-N-CA	6.28	125.92	121.65
57	BA	2502	G	O4'-C4'-C3'	6.28	110.28	104.00
22	AA	279	A	C4'-C3'-O3'	6.27	118.81	109.40
57	BA	2061	G	C4'-C3'-C2'	-6.27	96.33	102.60
25	BC	172	HIS	CA-CB-CG	6.24	120.03	113.80
57	BA	771	G	C5'-C4'-C3'	-6.23	106.65	116.00
57	BA	1943	U	O4'-C1'-N1	6.23	117.54	108.20
58	Ba	26	C	C5'-C4'-C3'	-6.22	106.67	116.00
24	A3	9	G	O4'-C1'-N9	6.19	117.49	108.20
22	AA	765	G	O4'-C1'-N9	6.19	117.49	108.20
57	BA	1064	C	C4'-C3'-C2'	-6.19	96.41	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	2312	U	O4'-C4'-C3'	6.18	110.18	104.00
46	B3	44	ARG	NE-CZ-NH2	6.17	124.76	119.20
57	BA	2472	G	C4'-C3'-C2'	-6.17	96.43	102.60
45	BE	83	ARG	NE-CZ-NH2	6.16	124.75	119.20
58	Ba	15	A	O4'-C1'-N9	6.16	117.44	108.20
57	BA	2204	G	C5'-C4'-C3'	-6.15	106.78	116.00
58	Ba	10	G	O4'-C4'-C3'	6.13	110.13	104.00
25	BC	180	PHE	CA-CB-CG	6.08	119.88	113.80
22	AA	415	A	O4'-C1'-N9	6.06	117.59	108.50
57	BA	604	G	C5'-C4'-C3'	-6.01	106.98	116.00
14	AC	231	ARG	NE-CZ-NH2	6.01	124.61	119.20
22	AA	1286	U	O4'-C1'-N1	6.00	117.20	108.20
57	BA	2576	G	O4'-C1'-N9	6.00	117.50	108.50
35	BD	52	HIS	CB-CG-CD2	-5.99	123.41	131.20
31	BQ	117	PHE	CA-CB-CG	5.98	119.78	113.80
43	B1	73	ARG	NE-CZ-NH2	5.98	124.58	119.20
22	AA	899	C	O4'-C1'-N1	5.97	117.46	108.50
26	BJ	55	ARG	NE-CZ-NH1	5.96	127.46	121.50
57	BA	1552	A	O4'-C1'-N9	5.94	117.40	108.50
53	BF	102	ARG	NE-CZ-NH2	5.92	124.53	119.20
57	BA	1653	G	C4'-C3'-O3'	5.92	118.28	109.40
22	AA	108	G	O4'-C1'-N9	5.92	117.38	108.50
22	AA	1253	G	C5'-C4'-C3'	-5.89	107.16	116.00
22	AA	422	C	O4'-C1'-N1	5.88	117.32	108.50
42	B0	28	GLU	CA-C-N	5.88	128.43	120.38
42	B0	28	GLU	C-N-CA	5.88	128.43	120.38
57	BA	2424	C	C3'-C2'-C1'	5.87	107.17	101.30
22	AA	356	A	C4'-C3'-C2'	-5.85	96.75	102.60
46	B3	10	ARG	NE-CZ-NH2	5.85	124.47	119.20
57	BA	2489	U	O4'-C4'-C3'	5.84	109.84	104.00
53	BF	49	ARG	NE-CZ-NH2	5.84	124.45	119.20
50	B7	16	HIS	CB-CG-CD2	-5.83	123.61	131.20
23	A2	24	A	C5'-C4'-C3'	-5.83	107.25	116.00
57	BA	914	G	C4'-C3'-C2'	-5.83	96.77	102.60
50	B7	34	ARG	CD-NE-CZ	5.79	132.51	124.40
22	AA	1050	G	C4'-C3'-C2'	-5.79	96.81	102.60
57	BA	1061	U	C4'-C3'-O3'	5.79	118.08	109.40
48	B5	51	ARG	NE-CZ-NH2	5.77	124.39	119.20
57	BA	2252	G	C2'-C3'-O3'	5.74	118.11	109.50
20	AI	109	GLN	OE1-CD-NE2	-5.74	116.86	122.60
22	AA	487	A	O4'-C4'-C3'	5.72	109.72	104.00
22	AA	531	U	C4'-C3'-O3'	5.72	117.98	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	1552	A	C1'-O4'-C4'	-5.72	104.18	109.90
18	AG	150	PHE	CA-CB-CG	5.71	119.51	113.80
57	BA	1566	A	O4'-C1'-N9	5.70	116.75	108.20
21	A1	483	TYR	CA-C-N	5.70	127.26	120.14
21	A1	483	TYR	C-N-CA	5.70	127.26	120.14
57	BA	2170	A	O4'-C4'-C3'	5.70	109.70	104.00
57	BA	2508	G	C4'-C3'-C2'	-5.69	96.91	102.60
57	BA	2755	C	O4'-C4'-C3'	5.69	109.69	104.00
22	AA	936	C	C4'-C3'-C2'	-5.68	96.92	102.60
22	AA	610	U	O4'-C1'-N1	5.68	117.02	108.50
22	AA	1502	A	O4'-C1'-N9	5.67	116.70	108.20
57	BA	2661	G	C2'-C3'-O3'	5.67	122.20	113.70
57	BA	2202	U	C4'-C3'-O3'	5.67	121.50	113.00
57	BA	782	A	C4'-C3'-O3'	5.66	117.89	109.40
57	BA	2662	A	C3'-C2'-C1'	5.66	107.16	101.50
57	BA	1674	G	O4'-C4'-C3'	5.66	109.66	104.00
43	B1	49	ARG	NE-CZ-NH2	5.65	124.29	119.20
57	BA	653	U	C2'-C3'-O3'	5.65	117.97	109.50
57	BA	750	A	O4'-C4'-C3'	5.65	109.65	104.00
57	BA	2799	A	O3'-P-O5'	5.65	112.47	104.00
22	AA	465	A	O4'-C1'-N9	5.64	116.66	108.20
57	BA	790	U	O4'-C1'-N1	5.64	116.66	108.20
57	BA	2023	C	C5'-C4'-C3'	-5.64	107.53	116.00
57	BA	1056	G	C2'-C3'-O3'	-5.64	105.24	113.70
57	BA	917	A	C5'-C4'-C3'	-5.64	107.55	116.00
22	AA	1268	G	O4'-C4'-C3'	5.63	109.63	104.00
22	AA	328	C	C4'-C3'-O3'	5.61	117.81	109.40
57	BA	449	A	O4'-C4'-C3'	5.60	109.60	104.00
57	BA	812	C	O4'-C4'-C3'	5.60	109.60	104.00
54	BG	101	ARG	NE-CZ-NH2	5.59	124.23	119.20
54	BG	109	ARG	NE-CZ-NH2	5.58	124.22	119.20
57	BA	866	A	O4'-C4'-C3'	5.58	109.58	104.00
43	B1	36	ARG	NE-CZ-NH2	5.57	124.22	119.20
22	AA	790	A	O4'-C4'-C3'	5.57	109.57	104.00
57	BA	414	C	C4'-C3'-C2'	-5.56	97.04	102.60
57	BA	2261	C	C5'-C4'-C3'	-5.56	107.66	116.00
57	BA	1624	U	C5'-C4'-C3'	-5.55	107.68	116.00
57	BA	1757	A	O4'-C4'-C3'	5.54	109.54	104.00
50	B7	19	ARG	NE-CZ-NH2	5.52	124.17	119.20
57	BA	13	A	C1'-O4'-C4'	-5.52	104.18	109.70
22	AA	522	C	O4'-C4'-C3'	5.52	109.52	104.00
57	BA	1622	G	O4'-C4'-C3'	5.51	109.52	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	793	U	C4'-C3'-C2'	-5.50	97.10	102.60
57	BA	1802	A	O4'-C4'-C3'	5.50	109.50	104.00
44	B2	52	ARG	NE-CZ-NH2	5.50	124.15	119.20
22	AA	1092	A	O4'-C4'-C3'	5.49	109.49	104.00
57	BA	2197	U	O3'-P-O5'	-5.49	95.77	104.00
11	AB	14	HIS	CB-CG-CD2	-5.48	124.07	131.20
22	AA	121	U	C3'-C2'-C1'	5.48	106.78	101.30
42	B0	13	ARG	NH1-CZ-NH2	-5.48	112.18	119.30
55	BH	2	ARG	NE-CZ-NH2	5.48	124.13	119.20
7	AP	70	ARG	NE-CZ-NH1	5.47	126.97	121.50
22	AA	1215	G	O4'-C4'-C3'	5.47	109.47	104.00
46	B3	24	LEU	CA-C-N	5.47	126.05	119.98
46	B3	24	LEU	C-N-CA	5.47	126.05	119.98
43	B1	17	ARG	NE-CZ-NH2	5.47	124.12	119.20
57	BA	2658	C	O3'-P-O5'	5.45	112.17	104.00
46	B3	29	ARG	NE-CZ-NH2	5.44	124.09	119.20
57	BA	526	A	O4'-C4'-C3'	5.44	109.44	104.00
57	BA	1789	A	O4'-C4'-C3'	5.44	109.44	104.00
45	BE	75	ALA	CA-C-N	5.43	125.26	120.10
45	BE	75	ALA	C-N-CA	5.43	125.26	120.10
15	AD	71	PHE	CA-CB-CG	5.43	119.23	113.80
22	AA	423	G	O4'-C1'-N9	5.43	116.64	108.50
22	AA	674	G	O4'-C4'-C3'	5.43	109.43	104.00
58	Ba	13	G	O4'-C4'-C3'	5.43	109.43	104.00
23	A2	24	A	O4'-C4'-C3'	5.42	109.42	104.00
28	BN	25	LEU	CA-C-N	5.42	125.96	120.00
28	BN	25	LEU	C-N-CA	5.42	125.96	120.00
57	BA	74	A	C5'-C4'-C3'	-5.42	107.07	115.20
57	BA	981	A	O4'-C4'-C3'	5.42	109.42	104.00
57	BA	2253	G	O4'-C1'-N9	5.42	116.33	108.20
53	BF	162	ARG	NE-CZ-NH2	5.42	124.08	119.20
57	BA	1648	U	C5'-C4'-C3'	-5.42	107.87	116.00
57	BA	804	A	C4'-C3'-O3'	5.41	117.52	109.40
57	BA	242	G	C1'-O4'-C4'	-5.41	104.29	109.70
57	BA	1013	C	C5'-C4'-C3'	-5.41	107.89	116.00
57	BA	1466	U	O3'-P-O5'	-5.41	95.89	104.00
13	AU	34	ARG	NH1-CZ-NH2	-5.41	112.27	119.30
50	B7	41	ARG	NE-CZ-NH2	5.40	124.06	119.20
22	AA	519	C	C2'-C3'-O3'	5.39	117.58	109.50
57	BA	2692	G	C4'-C3'-C2'	-5.38	97.22	102.60
22	AA	245	U	O4'-C4'-C3'	5.38	109.38	104.00
57	BA	2731	G	C5'-C4'-C3'	-5.38	107.94	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	816	C	C5'-C4'-C3'	-5.37	107.94	116.00
57	BA	1314	C	O4'-C4'-C3'	5.37	109.37	104.00
22	AA	729	A	C4'-C3'-C2'	-5.36	97.24	102.60
45	BE	128	ARG	NH1-CZ-NH2	-5.36	112.33	119.30
22	AA	1074	G	C5'-C4'-C3'	-5.36	107.97	116.00
57	BA	2275	C	C2'-C3'-O3'	-5.35	105.67	113.70
22	AA	346	G	O4'-C4'-C3'	5.35	109.35	104.00
57	BA	1021	A	C5'-C4'-C3'	-5.35	107.97	116.00
39	BX	70	HIS	CB-CG-CD2	-5.35	124.24	131.20
37	BV	91	GLN	OE1-CD-NE2	-5.34	117.26	122.60
57	BA	1508	A	O4'-C1'-N9	5.34	116.21	108.20
34	BT	108	ARG	NE-CZ-NH2	5.34	124.01	119.20
46	B3	15	ARG	NH1-CZ-NH2	-5.34	112.36	119.30
36	BU	32	ARG	NE-CZ-NH2	5.33	124.00	119.20
48	B5	15	ARG	NE-CZ-NH2	5.33	124.00	119.20
24	A3	16	C	O4'-C1'-N1	5.33	116.19	108.20
22	AA	381	C	O4'-C1'-N1	5.32	116.18	108.20
35	BD	238	ASN	OD1-CG-ND2	-5.32	117.28	122.60
57	BA	2061	G	P-O3'-C3'	5.31	128.17	120.20
22	AA	331	G	C2'-C3'-O3'	5.31	117.47	109.50
13	AU	34	ARG	NE-CZ-NH1	5.31	126.81	121.50
54	BG	91	ARG	NE-CZ-NH2	5.31	123.98	119.20
58	Ba	90	C	C5'-C4'-C3'	-5.31	108.04	116.00
57	BA	359	G	C2'-C3'-O3'	5.30	117.46	109.50
57	BA	506	G	C4'-C3'-O3'	5.30	117.36	109.40
50	B7	12	ARG	NE-CZ-NH2	5.30	123.97	119.20
22	AA	965	U	O4'-C1'-N1	5.30	116.15	108.20
57	BA	33	C	O3'-P-O5'	-5.30	96.05	104.00
31	BQ	44	ARG	NE-CZ-NH2	5.30	123.97	119.20
22	AA	692	U	O4'-C4'-C3'	5.29	109.29	104.00
57	BA	2874	C	O4'-C4'-C3'	5.29	109.29	104.00
11	AB	161	PHE	CA-CB-CG	5.29	119.09	113.80
22	AA	251	G	O4'-C1'-N9	5.28	116.12	108.20
22	AA	1296	C	O4'-C4'-C3'	5.28	109.28	104.00
22	AA	1079	G	O4'-C4'-C3'	5.28	109.28	104.00
57	BA	37	C	C4'-C3'-C2'	-5.27	97.33	102.60
46	B3	15	ARG	NE-CZ-NH2	5.27	123.94	119.20
22	AA	719	C	O4'-C4'-C3'	5.27	109.27	104.00
57	BA	2777	G	O4'-C4'-C3'	5.27	109.27	104.00
22	AA	509	A	O4'-C4'-C3'	5.26	109.27	104.00
57	BA	2892	G	C5'-C4'-C3'	-5.26	107.30	115.20
57	BA	112	U	C4'-C3'-C2'	-5.26	97.34	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	573	U	C5'-C4'-C3'	-5.26	107.32	115.20
57	BA	712	G	C4'-C3'-C2'	-5.26	97.34	102.60
57	BA	715	A	O4'-C4'-C3'	5.26	109.26	104.00
57	BA	1452	G	O4'-C4'-C3'	5.26	109.26	104.00
45	BE	59	ARG	NE-CZ-NH2	5.25	123.93	119.20
57	BA	900	A	C2'-C3'-O3'	5.25	117.38	109.50
22	AA	1119	C	C5'-C4'-C3'	-5.25	108.12	116.00
57	BA	729	G	C5'-C4'-C3'	-5.25	108.12	116.00
57	BA	1398	C	O4'-C4'-C3'	5.25	109.25	104.00
22	AA	845	A	C2'-C3'-O3'	5.24	117.36	109.50
22	AA	307	C	O3'-P-O5'	5.24	111.86	104.00
22	AA	1179	A	O4'-C4'-C3'	5.24	109.24	104.00
57	BA	1098	A	C5'-C4'-C3'	-5.24	108.15	116.00
22	AA	573	A	O4'-C4'-C3'	5.23	109.23	104.00
44	B2	7	ARG	NH1-CZ-NH2	-5.23	112.51	119.30
53	BF	102	ARG	NE-CZ-NH1	-5.21	116.29	121.50
43	B1	10	ARG	NE-CZ-NH2	5.21	123.89	119.20
57	BA	2243	U	C5'-C4'-C3'	-5.21	108.19	116.00
57	BA	2309	A	C2'-C3'-O3'	5.21	117.31	109.50
57	BA	2450	A	C5'-C4'-C3'	-5.21	108.19	116.00
57	BA	2134	A	O4'-C1'-N9	5.20	116.31	108.50
57	BA	2054	A	C5'-C4'-C3'	-5.20	108.20	116.00
20	AI	80	HIS	CB-CG-CD2	-5.20	124.44	131.20
22	AA	412	A	C1'-O4'-C4'	-5.20	104.50	109.70
57	BA	1029	A	C5'-C4'-C3'	-5.20	108.20	116.00
30	BP	33	ARG	NE-CZ-NH1	5.19	126.69	121.50
31	BQ	81	ARG	NE-CZ-NH1	5.19	126.69	121.50
22	AA	1220	G	C4'-C3'-C2'	-5.19	97.41	102.60
31	BQ	10	ARG	NE-CZ-NH2	5.19	123.87	119.20
22	AA	120	A	O4'-C4'-C3'	5.18	109.18	104.00
53	BF	88	ARG	NE-CZ-NH2	5.18	123.86	119.20
57	BA	819	A	C5'-C4'-C3'	-5.18	108.23	116.00
57	BA	1313	U	O4'-C4'-C3'	5.18	109.18	104.00
37	BV	78	ARG	NE-CZ-NH2	5.17	123.86	119.20
45	BE	169	ARG	NE-CZ-NH2	5.17	123.86	119.20
57	BA	1606	C	C4'-C3'-C2'	-5.17	97.43	102.60
22	AA	496	A	C1'-O4'-C4'	-5.16	104.74	109.90
28	BN	120	ARG	NE-CZ-NH2	5.16	123.85	119.20
22	AA	382	A	O4'-C4'-C3'	5.16	109.16	104.00
22	AA	1322	C	O4'-C1'-N1	5.16	115.94	108.20
53	BF	41	GLN	CA-C-N	5.15	124.87	119.92
53	BF	41	GLN	C-N-CA	5.15	124.87	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	2076	U	C4'-C3'-O3'	5.15	120.73	113.00
23	A2	23	C	O4'-C4'-C3'	5.15	109.15	104.00
57	BA	422	A	O4'-C4'-C3'	5.15	109.15	104.00
38	BW	88	ARG	NE-CZ-NH2	5.14	123.83	119.20
27	BK	23	VAL	CA-C-N	5.14	124.88	121.13
27	BK	23	VAL	C-N-CA	5.14	124.88	121.13
57	BA	2615	U	O4'-C4'-C3'	5.14	109.14	104.00
23	A2	54	U	O4'-C4'-C3'	5.14	109.14	104.00
22	AA	1093	A	O4'-C4'-C3'	5.13	109.14	104.00
22	AA	493	A	C3'-C2'-C1'	5.13	106.43	101.30
22	AA	843	U	O4'-C1'-N1	5.13	115.89	108.20
57	BA	1927	A	O4'-C4'-C3'	5.13	109.13	104.00
57	BA	2424	C	C1'-O4'-C4'	-5.13	104.77	109.90
57	BA	523	C	C4'-C3'-C2'	-5.13	97.47	102.60
57	BA	971	G	C5'-C4'-C3'	-5.13	108.31	116.00
57	BA	429	A	O4'-C4'-C3'	5.12	109.12	104.00
23	A2	45	G	C3'-C2'-C1'	5.12	106.42	101.30
57	BA	2252	G	O3'-P-O5'	-5.12	96.32	104.00
22	AA	51	A	C4'-C3'-O3'	5.12	117.08	109.40
57	BA	2321	U	O3'-P-O5'	-5.12	96.33	104.00
22	AA	1014	A	O4'-C4'-C3'	5.11	109.11	104.00
57	BA	716	A	C5'-C4'-C3'	-5.11	108.33	116.00
57	BA	1263	U	C5'-C4'-C3'	-5.11	108.33	116.00
29	BO	76	VAL	N-CA-C	5.11	115.63	108.89
22	AA	1221	G	C4'-C3'-C2'	-5.11	97.49	102.60
57	BA	1251	C	C1'-O4'-C4'	-5.10	104.80	109.90
57	BA	914	G	C2'-C3'-O3'	5.10	117.15	109.50
22	AA	675	A	C5'-C4'-C3'	-5.09	108.36	116.00
57	BA	210	C	C5'-C4'-C3'	-5.09	108.36	116.00
35	BD	199	HIS	CB-CG-CD2	-5.09	124.58	131.20
38	BW	102	HIS	CB-CG-CD2	-5.09	124.58	131.20
22	AA	1469	C	O4'-C4'-C3'	5.09	109.09	104.00
57	BA	2885	G	C2'-C3'-O3'	-5.09	106.07	113.70
57	BA	1864	U	O4'-C4'-C3'	5.08	109.08	104.00
57	BA	586	A	O4'-C4'-C3'	5.08	109.08	104.00
57	BA	2757	A	C5'-C4'-C3'	-5.08	108.38	116.00
57	BA	2766	A	O4'-C4'-C3'	5.08	109.08	104.00
22	AA	619	U	O4'-C4'-C3'	5.07	109.07	104.00
53	BF	97	ASN	CA-CB-CG	5.07	117.67	112.60
57	BA	2660	A	C3'-C2'-C1'	5.07	106.37	101.30
57	BA	2831	G	C5'-C4'-C3'	-5.07	108.40	116.00
23	A2	51	C	O4'-C4'-C3'	5.07	109.07	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	731	G	C4'-C3'-C2'	-5.06	97.54	102.60
57	BA	190	A	C4'-C3'-C2'	-5.06	97.54	102.60
57	BA	335	C	O4'-C4'-C3'	5.06	109.06	104.00
23	A2	27	A	C4'-C3'-C2'	-5.06	97.54	102.60
57	BA	2725	A	C2'-C3'-O3'	5.06	117.08	109.50
57	BA	952	G	C5'-C4'-C3'	-5.05	108.42	116.00
16	AE	88	HIS	CB-CG-CD2	-5.05	124.64	131.20
43	B1	56	ARG	NE-CZ-NH2	5.05	123.74	119.20
57	BA	409	G	C4'-C3'-C2'	-5.05	97.55	102.60
57	BA	301	G	C4'-C3'-C2'	-5.05	97.55	102.60
41	BZ	88	HIS	CB-CG-CD2	-5.04	124.64	131.20
27	BK	21	PRO	N-CA-C	5.04	116.85	110.70
35	BD	220	ARG	NH1-CZ-NH2	-5.04	112.74	119.30
50	B7	3	ARG	NE-CZ-NH2	5.04	123.74	119.20
22	AA	1318	A	O4'-C4'-C3'	5.04	109.04	104.00
57	BA	1611	C	O4'-C4'-C3'	5.04	109.04	104.00
22	AA	872	A	C1'-O4'-C4'	-5.04	104.66	109.70
57	BA	1187	G	O4'-C4'-C3'	5.04	109.04	104.00
57	BA	2090	A	O3'-P-O5'	5.04	111.55	104.00
58	Ba	88	C	C2'-C3'-O3'	5.03	117.04	109.50
22	AA	504	C	C5'-C4'-C3'	-5.02	108.47	116.00
39	BX	13	ALA	N-CA-C	5.01	112.73	108.22
57	BA	2565	A	C2'-C3'-O3'	5.01	117.02	109.50
1	AJ	56	HIS	CA-C-N	5.01	130.72	121.70
1	AJ	56	HIS	C-N-CA	5.01	130.72	121.70
57	BA	2245	U	O3'-P-O5'	-5.01	96.49	104.00
10	AS	77	ARG	NH1-CZ-NH2	-5.01	112.79	119.30
57	BA	255	A	C5'-C4'-C3'	-5.00	108.49	116.00
21	A1	492	TRP	CA-C-N	5.00	131.09	121.54
21	A1	492	TRP	C-N-CA	5.00	131.09	121.54

There are no chirality outliers.

All (1070) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	A1	289	ILE	Peptide
21	A1	374	LEU	Peptide
23	A2	23	C	Sidechain
23	A2	34	U	Sidechain
23	A2	39	U	Sidechain
23	A2	44	U	Sidechain
23	A2	45	G	Sidechain

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Mol	Chain	Res	Type	Group
24	A3	1	C	Sidechain
24	A3	14	A	Sidechain
24	A3	15	G	Sidechain
24	A3	20	G	Sidechain
24	A3	23	G	Sidechain
24	A3	28	U	Sidechain
24	A3	30	G	Sidechain
24	A3	40	C	Sidechain
24	A3	46	G	Sidechain
24	A3	47	A	Sidechain
24	A3	60	A	Sidechain
24	A3	64	G	Sidechain
24	A3	65	G	Sidechain
24	A3	69	C	Sidechain
24	A3	7	G	Sidechain
22	AA	100	G	Sidechain
22	AA	1008	U	Sidechain
22	AA	1010	U	Sidechain
22	AA	1013	G	Sidechain
22	AA	1016	A	Sidechain
22	AA	1026	G	Sidechain
22	AA	1027	C	Sidechain
22	AA	1028	C	Sidechain
22	AA	1030	U	Sidechain
22	AA	1032	G	Sidechain
22	AA	1051	C	Sidechain
22	AA	1054	C	Sidechain
22	AA	1067	A	Sidechain
22	AA	1071	C	Sidechain
22	AA	1072	G	Sidechain
22	AA	1077	G	Sidechain
22	AA	1080	A	Sidechain
22	AA	1082	A	Sidechain
22	AA	1084	G	Sidechain
22	AA	1087	G	Sidechain
22	AA	1093	A	Sidechain
22	AA	1094	G	Sidechain
22	AA	1095	U	Sidechain
22	AA	1099	G	Sidechain
22	AA	110	C	Sidechain
22	AA	1100	C	Sidechain
22	AA	1101	A	Sidechain

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Mol	Chain	Res	Type	Group
22	AA	1109	C	Sidechain
22	AA	1111	A	Sidechain
22	AA	1112	C	Sidechain
22	AA	1114	C	Sidechain
22	AA	1115	U	Sidechain
22	AA	1117	A	Sidechain
22	AA	1118	U	Sidechain
22	AA	1120	C	Sidechain
22	AA	1122	U	Sidechain
22	AA	1131	G	Sidechain
22	AA	1139	G	Sidechain
22	AA	1142	G	Sidechain
22	AA	1148	U	Sidechain
22	AA	1149	C	Sidechain
22	AA	1153	G	Sidechain
22	AA	1155	A	Sidechain
22	AA	1157	A	Sidechain
22	AA	1160	G	Sidechain
22	AA	1169	A	Sidechain
22	AA	117	G	Sidechain
22	AA	1170	A	Sidechain
22	AA	1176	A	Sidechain
22	AA	1178	G	Sidechain
22	AA	1179	A	Sidechain
22	AA	119	A	Sidechain
22	AA	1191	A	Sidechain
22	AA	1195	C	Sidechain
22	AA	1209	C	Sidechain
22	AA	121	U	Sidechain
22	AA	1213	A	Sidechain
22	AA	1225	A	Sidechain
22	AA	1226	C	Sidechain
22	AA	1233	G	Sidechain
22	AA	1234	C	Sidechain
22	AA	1240	U	Sidechain
22	AA	1250	A	Sidechain
22	AA	1251	A	Sidechain
22	AA	1264	U	Sidechain
22	AA	1266	G	Sidechain
22	AA	1267	C	Sidechain
22	AA	1269	A	Sidechain
22	AA	1278	G	Sidechain

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Mol	Chain	Res	Type	Group
22	AA	128	G	Sidechain
22	AA	1282	C	Sidechain
22	AA	1287	A	Sidechain
22	AA	1289	A	Sidechain
22	AA	1296	C	Sidechain
22	AA	1297	G	Sidechain
22	AA	1298	U	Sidechain
22	AA	1299	A	Sidechain
22	AA	130	A	Sidechain
22	AA	1300	G	Sidechain
22	AA	1303	C	Sidechain
22	AA	1304	G	Sidechain
22	AA	1305	G	Sidechain
22	AA	1306	A	Sidechain
22	AA	1308	U	Sidechain
22	AA	1316	G	Sidechain
22	AA	1317	C	Sidechain
22	AA	1319	A	Sidechain
22	AA	1326	U	Sidechain
22	AA	1330	U	Sidechain
22	AA	1343	G	Sidechain
22	AA	1345	U	Sidechain
22	AA	1349	A	Sidechain
22	AA	1357	A	Sidechain
22	AA	1358	U	Sidechain
22	AA	1360	A	Sidechain
22	AA	1361	G	Sidechain
22	AA	1362	A	Sidechain
22	AA	1363	A	Sidechain
22	AA	1366	C	Sidechain
22	AA	1373	G	Sidechain
22	AA	1374	A	Sidechain
22	AA	1380	U	Sidechain
22	AA	1382	C	Sidechain
22	AA	1392	G	Sidechain
22	AA	1394	A	Sidechain
22	AA	1396	A	Sidechain
22	AA	1400	C	Sidechain
22	AA	1401	G	Sidechain
22	AA	1411	C	Sidechain
22	AA	1419	G	Sidechain
22	AA	1426	G	Sidechain

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Mol	Chain	Res	Type	Group
22	AA	143	A	Sidechain
22	AA	1430	A	Sidechain
22	AA	1432	G	Sidechain
22	AA	1433	A	Sidechain
22	AA	1447	A	Sidechain
22	AA	1448	C	Sidechain
22	AA	1449	C	Sidechain
22	AA	1451	U	Sidechain
22	AA	1453	G	Sidechain
22	AA	1468	A	Sidechain
22	AA	1477	U	Sidechain
22	AA	1489	G	Sidechain
22	AA	149	A	Sidechain
22	AA	1490	U	Sidechain
22	AA	1502	A	Sidechain
22	AA	1503	A	Sidechain
22	AA	1506	U	Sidechain
22	AA	1512	U	Sidechain
22	AA	1513	A	Sidechain
22	AA	1517	G	Sidechain
22	AA	1528	U	Sidechain
22	AA	153	C	Sidechain
22	AA	1535	C	Sidechain
22	AA	1537	U	Sidechain
22	AA	1542	A	Sidechain
22	AA	158	G	Sidechain
22	AA	159	G	Sidechain
22	AA	161	A	Sidechain
22	AA	173	U	Sidechain
22	AA	179	A	Sidechain
22	AA	182	A	Sidechain
22	AA	184	G	Sidechain
22	AA	187	G	Sidechain
22	AA	188	C	Sidechain
22	AA	2	A	Sidechain
22	AA	201	G	Sidechain
22	AA	202	G	Sidechain
22	AA	205	A	Sidechain
22	AA	209	U	Sidechain
22	AA	21	G	Sidechain
22	AA	212	G	Sidechain
22	AA	214	C	Sidechain

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Mol	Chain	Res	Type	Group
22	AA	215	C	Sidechain
22	AA	217	C	Sidechain
22	AA	222	C	Sidechain
22	AA	223	A	Sidechain
22	AA	234	C	Sidechain
22	AA	236	A	Sidechain
22	AA	244	U	Sidechain
22	AA	245	U	Sidechain
22	AA	246	A	Sidechain
22	AA	249	U	Sidechain
22	AA	252	U	Sidechain
22	AA	262	A	Sidechain
22	AA	264	C	Sidechain
22	AA	268	U	Sidechain
22	AA	269	C	Sidechain
22	AA	270	A	Sidechain
22	AA	272	C	Sidechain
22	AA	278	G	Sidechain
22	AA	279	A	Sidechain
22	AA	281	G	Sidechain
22	AA	282	A	Sidechain
22	AA	285	C	Sidechain
22	AA	286	C	Sidechain
22	AA	293	G	Sidechain
22	AA	3	A	Sidechain
22	AA	304	U	Sidechain
22	AA	306	A	Sidechain
22	AA	308	C	Sidechain
22	AA	313	A	Sidechain
22	AA	314	C	Sidechain
22	AA	316	C	Sidechain
22	AA	324	G	Sidechain
22	AA	325	A	Sidechain
22	AA	33	A	Sidechain
22	AA	330	C	Sidechain
22	AA	332	G	Sidechain
22	AA	333	U	Sidechain
22	AA	336	A	Sidechain
22	AA	345	C	Sidechain
22	AA	346	G	Sidechain
22	AA	354	G	Sidechain
22	AA	36	C	Sidechain

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Mol	Chain	Res	Type	Group
22	AA	362	G	Sidechain
22	AA	368	U	Sidechain
22	AA	371	A	Sidechain
22	AA	376	G	Sidechain
22	AA	380	G	Sidechain
22	AA	383	A	Sidechain
22	AA	387	U	Sidechain
22	AA	390	U	Sidechain
22	AA	391	G	Sidechain
22	AA	392	C	Sidechain
22	AA	394	G	Sidechain
22	AA	395	C	Sidechain
22	AA	404	G	Sidechain
22	AA	410	G	Sidechain
22	AA	42	G	Sidechain
22	AA	423	G	Sidechain
22	AA	426	U	Sidechain
22	AA	428	G	Sidechain
22	AA	429	U	Sidechain
22	AA	442	G	Sidechain
22	AA	448	A	Sidechain
22	AA	455	G	Sidechain
22	AA	457	G	Sidechain
22	AA	459	A	Sidechain
22	AA	46	G	Sidechain
22	AA	460	A	Sidechain
22	AA	463	U	Sidechain
22	AA	469	C	Sidechain
22	AA	472	U	Sidechain
22	AA	48	C	Sidechain
22	AA	481	G	Sidechain
22	AA	488	C	Sidechain
22	AA	490	C	Sidechain
22	AA	491	G	Sidechain
22	AA	493	A	Sidechain
22	AA	506	G	Sidechain
22	AA	51	A	Sidechain
22	AA	517	G	Sidechain
22	AA	518	C	Sidechain
22	AA	521	G	Sidechain
22	AA	522	C	Sidechain
22	AA	529	G	Sidechain

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Mol	Chain	Res	Type	Group
22	AA	530	G	Sidechain
22	AA	534	U	Sidechain
22	AA	535	A	Sidechain
22	AA	540	G	Sidechain
22	AA	551	U	Sidechain
22	AA	554	A	Sidechain
22	AA	558	G	Sidechain
22	AA	56	U	Sidechain
22	AA	560	A	Sidechain
22	AA	562	U	Sidechain
22	AA	563	A	Sidechain
22	AA	566	G	Sidechain
22	AA	568	G	Sidechain
22	AA	572	A	Sidechain
22	AA	590	U	Sidechain
22	AA	592	G	Sidechain
22	AA	594	U	Sidechain
22	AA	595	A	Sidechain
22	AA	597	G	Sidechain
22	AA	60	A	Sidechain
22	AA	600	A	Sidechain
22	AA	608	A	Sidechain
22	AA	612	C	Sidechain
22	AA	618	C	Sidechain
22	AA	620	C	Sidechain
22	AA	623	C	Sidechain
22	AA	631	C	Sidechain
22	AA	639	G	Sidechain
22	AA	640	A	Sidechain
22	AA	641	U	Sidechain
22	AA	642	A	Sidechain
22	AA	654	G	Sidechain
22	AA	664	G	Sidechain
22	AA	665	A	Sidechain
22	AA	666	G	Sidechain
22	AA	67	C	Sidechain
22	AA	676	A	Sidechain
22	AA	679	C	Sidechain
22	AA	686	U	Sidechain
22	AA	690	G	Sidechain
22	AA	691	G	Sidechain
22	AA	692	U	Sidechain

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Mol	Chain	Res	Type	Group
22	AA	695	A	Sidechain
22	AA	697	U	Sidechain
22	AA	70	U	Sidechain
22	AA	703	G	Sidechain
22	AA	71	A	Sidechain
22	AA	722	G	Sidechain
22	AA	725	G	Sidechain
22	AA	728	A	Sidechain
22	AA	737	C	Sidechain
22	AA	745	G	Sidechain
22	AA	752	G	Sidechain
22	AA	754	C	Sidechain
22	AA	761	G	Sidechain
22	AA	771	G	Sidechain
22	AA	775	G	Sidechain
22	AA	778	G	Sidechain
22	AA	779	C	Sidechain
22	AA	781	A	Sidechain
22	AA	788	U	Sidechain
22	AA	790	A	Sidechain
22	AA	791	G	Sidechain
22	AA	793	U	Sidechain
22	AA	795	C	Sidechain
22	AA	8	A	Sidechain
22	AA	80	A	Sidechain
22	AA	802	A	Sidechain
22	AA	805	C	Sidechain
22	AA	811	C	Sidechain
22	AA	816	A	Sidechain
22	AA	824	G	Sidechain
22	AA	826	C	Sidechain
22	AA	828	U	Sidechain
22	AA	838	G	Sidechain
22	AA	842	U	Sidechain
22	AA	843	U	Sidechain
22	AA	855	U	Sidechain
22	AA	859	G	Sidechain
22	AA	860	A	Sidechain
22	AA	863	U	Sidechain
22	AA	864	A	Sidechain
22	AA	87	C	Sidechain
22	AA	872	A	Sidechain

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Mol	Chain	Res	Type	Group
22	AA	874	G	Sidechain
22	AA	883	C	Sidechain
22	AA	892	A	Sidechain
22	AA	898	G	Sidechain
22	AA	900	A	Sidechain
22	AA	906	A	Sidechain
22	AA	91	U	Sidechain
22	AA	912	C	Sidechain
22	AA	914	A	Sidechain
22	AA	937	A	Sidechain
22	AA	938	A	Sidechain
22	AA	939	G	Sidechain
22	AA	94	G	Sidechain
22	AA	942	G	Sidechain
22	AA	946	A	Sidechain
22	AA	949	A	Sidechain
22	AA	95	C	Sidechain
22	AA	951	G	Sidechain
22	AA	958	A	Sidechain
22	AA	960	U	Sidechain
22	AA	961	U	Sidechain
22	AA	962	C	Sidechain
22	AA	971	G	Sidechain
22	AA	972	C	Sidechain
22	AA	979	C	Sidechain
22	AA	985	C	Sidechain
22	AA	99	C	Sidechain
22	AA	991	U	Sidechain
22	AA	997	U	Sidechain
15	AD	61	ARG	Sidechain
18	AG	101	ARG	Sidechain
18	AG	118	ARG	Sidechain
3	AL	109	ARG	Sidechain
6	AO	88	ARG	Sidechain
7	AP	25	ARG	Sidechain
9	AR	2	ARG	Sidechain
10	AS	79	TYR	Sidechain
42	B0	54	ARG	Sidechain
51	B8	12	ARG	Sidechain
57	BA	100	U	Sidechain
57	BA	1004	U	Sidechain
57	BA	1012	U	Sidechain

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Mol	Chain	Res	Type	Group
57	BA	1013	C	Sidechain
57	BA	1014	A	Sidechain
57	BA	1017	G	Sidechain
57	BA	102	U	Sidechain
57	BA	1025	G	Sidechain
57	BA	1026	G	Sidechain
57	BA	1027	A	Sidechain
57	BA	1028	A	Sidechain
57	BA	103	A	Sidechain
57	BA	104	A	Sidechain
57	BA	1045	C	Sidechain
57	BA	1046	A	Sidechain
57	BA	1047	G	Sidechain
57	BA	1048	A	Sidechain
57	BA	1050	A	Sidechain
57	BA	1057	A	Sidechain
57	BA	106	C	Sidechain
57	BA	1063	G	Sidechain
57	BA	1066	U	Sidechain
57	BA	1069	A	Sidechain
57	BA	107	G	Sidechain
57	BA	1071	G	Sidechain
57	BA	1072	C	Sidechain
57	BA	1075	C	Sidechain
57	BA	1081	U	Sidechain
57	BA	1082	U	Sidechain
57	BA	1083	U	Sidechain
57	BA	1085	A	Sidechain
57	BA	1088	A	Sidechain
57	BA	109	C	Sidechain
57	BA	1095	A	Sidechain
57	BA	1097	U	Sidechain
57	BA	1099	G	Sidechain
57	BA	1104	C	Sidechain
57	BA	1108	U	Sidechain
57	BA	1111	A	Sidechain
57	BA	1119	U	Sidechain
57	BA	1130	U	Sidechain
57	BA	1132	U	Sidechain
57	BA	1133	A	Sidechain
57	BA	1134	A	Sidechain
57	BA	1135	C	Sidechain

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Mol	Chain	Res	Type	Group
57	BA	1138	G	Sidechain
57	BA	1142	A	Sidechain
57	BA	1148	U	Sidechain
57	BA	1158	C	Sidechain
57	BA	1165	A	Sidechain
57	BA	1167	C	Sidechain
57	BA	1168	G	Sidechain
57	BA	1169	A	Sidechain
57	BA	1171	G	Sidechain
57	BA	1174	U	Sidechain
57	BA	1177	G	Sidechain
57	BA	1178	C	Sidechain
57	BA	1179	G	Sidechain
57	BA	1182	G	Sidechain
57	BA	1187	G	Sidechain
57	BA	1188	U	Sidechain
57	BA	1189	A	Sidechain
57	BA	1198	U	Sidechain
57	BA	12	U	Sidechain
57	BA	1200	C	Sidechain
57	BA	1202	G	Sidechain
57	BA	1205	A	Sidechain
57	BA	1206	G	Sidechain
57	BA	1209	U	Sidechain
57	BA	1210	G	Sidechain
57	BA	1223	G	Sidechain
57	BA	1225	G	Sidechain
57	BA	1226	A	Sidechain
57	BA	1227	G	Sidechain
57	BA	1230	A	Sidechain
57	BA	1232	G	Sidechain
57	BA	1236	G	Sidechain
57	BA	1238	G	Sidechain
57	BA	124	G	Sidechain
57	BA	1245	G	Sidechain
57	BA	1251	C	Sidechain
57	BA	1252	G	Sidechain
57	BA	1254	A	Sidechain
57	BA	1255	U	Sidechain
57	BA	1263	U	Sidechain
57	BA	1267	U	Sidechain
57	BA	1268	A	Sidechain

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Mol	Chain	Res	Type	Group
57	BA	1271	G	Sidechain
57	BA	1273	U	Sidechain
57	BA	1281	G	Sidechain
57	BA	1283	G	Sidechain
57	BA	1288	G	Sidechain
57	BA	1291	C	Sidechain
57	BA	1299	G	Sidechain
57	BA	1302	A	Sidechain
57	BA	1310	G	Sidechain
57	BA	1311	G	Sidechain
57	BA	1315	C	Sidechain
57	BA	1324	G	Sidechain
57	BA	1329	U	Sidechain
57	BA	1343	G	Sidechain
57	BA	1353	A	Sidechain
57	BA	1356	G	Sidechain
57	BA	1364	G	Sidechain
57	BA	1370	C	Sidechain
57	BA	1376	C	Sidechain
57	BA	1377	G	Sidechain
57	BA	1378	A	Sidechain
57	BA	138	U	Sidechain
57	BA	1398	C	Sidechain
57	BA	1402	U	Sidechain
57	BA	1405	U	Sidechain
57	BA	1406	U	Sidechain
57	BA	1410	G	Sidechain
57	BA	1425	G	Sidechain
57	BA	1427	A	Sidechain
57	BA	1431	A	Sidechain
57	BA	144	A	Sidechain
57	BA	1450	G	Sidechain
57	BA	146	A	Sidechain
57	BA	1464	G	Sidechain
57	BA	1465	G	Sidechain
57	BA	1467	U	Sidechain
57	BA	1469	A	Sidechain
57	BA	1473	G	Sidechain
57	BA	1474	U	Sidechain
57	BA	1482	G	Sidechain
57	BA	1483	G	Sidechain
57	BA	1492	G	Sidechain

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Mol	Chain	Res	Type	Group
57	BA	1494	A	Sidechain
57	BA	1495	A	Sidechain
57	BA	1508	A	Sidechain
57	BA	1517	G	Sidechain
57	BA	152	A	Sidechain
57	BA	1532	A	Sidechain
57	BA	1535	A	Sidechain
57	BA	1537	G	Sidechain
57	BA	1544	A	Sidechain
57	BA	1546	G	Sidechain
57	BA	1548	A	Sidechain
57	BA	1549	A	Sidechain
57	BA	1551	A	Sidechain
57	BA	1554	U	Sidechain
57	BA	1555	G	Sidechain
57	BA	1560	G	Sidechain
57	BA	1561	C	Sidechain
57	BA	1564	C	Sidechain
57	BA	1569	A	Sidechain
57	BA	1570	A	Sidechain
57	BA	1573	G	Sidechain
57	BA	1575	C	Sidechain
57	BA	1583	A	Sidechain
57	BA	1596	A	Sidechain
57	BA	1599	U	Sidechain
57	BA	160	A	Sidechain
57	BA	1601	G	Sidechain
57	BA	1602	U	Sidechain
57	BA	1606	C	Sidechain
57	BA	1610	A	Sidechain
57	BA	1616	A	Sidechain
57	BA	1627	G	Sidechain
57	BA	1630	A	Sidechain
57	BA	1631	G	Sidechain
57	BA	1632	A	Sidechain
57	BA	1639	C	Sidechain
57	BA	1641	A	Sidechain
57	BA	1643	G	Sidechain
57	BA	1645	G	Sidechain
57	BA	1650	A	Sidechain
57	BA	1651	G	Sidechain
57	BA	1652	A	Sidechain

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Mol	Chain	Res	Type	Group
57	BA	1653	G	Sidechain
57	BA	1656	C	Sidechain
57	BA	1663	G	Sidechain
57	BA	1667	G	Sidechain
57	BA	1671	U	Sidechain
57	BA	1672	A	Sidechain
57	BA	1680	U	Sidechain
57	BA	1681	G	Sidechain
57	BA	1682	G	Sidechain
57	BA	1687	G	Sidechain
57	BA	169	G	Sidechain
57	BA	1695	G	Sidechain
57	BA	1698	A	Sidechain
57	BA	17	G	Sidechain
57	BA	1701	A	Sidechain
57	BA	1704	C	Sidechain
57	BA	1705	A	Sidechain
57	BA	1706	C	Sidechain
57	BA	1708	C	Sidechain
57	BA	1710	G	Sidechain
57	BA	1713	A	Sidechain
57	BA	1721	G	Sidechain
57	BA	1726	C	Sidechain
57	BA	1736	U	Sidechain
57	BA	1739	A	Sidechain
57	BA	1744	A	Sidechain
57	BA	1745	A	Sidechain
57	BA	1749	A	Sidechain
57	BA	1750	G	Sidechain
57	BA	1761	C	Sidechain
57	BA	1762	A	Sidechain
57	BA	177	G	Sidechain
57	BA	1773	A	Sidechain
57	BA	1786	A	Sidechain
57	BA	179	C	Sidechain
57	BA	1797	G	Sidechain
57	BA	1798	U	Sidechain
57	BA	1799	G	Sidechain
57	BA	1802	A	Sidechain
57	BA	1805	A	Sidechain
57	BA	1807	G	Sidechain
57	BA	181	A	Sidechain

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Mol	Chain	Res	Type	Group
57	BA	1818	U	Sidechain
57	BA	182	A	Sidechain
57	BA	1821	A	Sidechain
57	BA	1830	C	Sidechain
57	BA	1831	G	Sidechain
57	BA	1842	G	Sidechain
57	BA	1848	A	Sidechain
57	BA	1851	U	Sidechain
57	BA	1857	G	Sidechain
57	BA	1865	U	Sidechain
57	BA	1866	A	Sidechain
57	BA	1869	G	Sidechain
57	BA	1870	C	Sidechain
57	BA	1881	C	Sidechain
57	BA	1883	U	Sidechain
57	BA	1885	A	Sidechain
57	BA	1900	A	Sidechain
57	BA	191	A	Sidechain
57	BA	1918	A	Sidechain
57	BA	1922	G	Sidechain
57	BA	1926	U	Sidechain
57	BA	1927	A	Sidechain
57	BA	1938	A	Sidechain
57	BA	194	G	Sidechain
57	BA	1941	C	Sidechain
57	BA	1945	G	Sidechain
57	BA	1948	G	Sidechain
57	BA	1952	A	Sidechain
57	BA	1953	A	Sidechain
57	BA	1970	A	Sidechain
57	BA	1972	G	Sidechain
57	BA	1973	G	Sidechain
57	BA	1976	U	Sidechain
57	BA	1982	U	Sidechain
57	BA	199	A	Sidechain
57	BA	1996	C	Sidechain
57	BA	1997	C	Sidechain
57	BA	2	G	Sidechain
57	BA	2002	G	Sidechain
57	BA	2007	U	Sidechain
57	BA	2011	U	Sidechain
57	BA	2012	G	Sidechain

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Mol	Chain	Res	Type	Group
57	BA	2019	A	Sidechain
57	BA	203	A	Sidechain
57	BA	2033	A	Sidechain
57	BA	2035	G	Sidechain
57	BA	2050	C	Sidechain
57	BA	2051	A	Sidechain
57	BA	2053	G	Sidechain
57	BA	2057	G	Sidechain
57	BA	2059	A	Sidechain
57	BA	2063	C	Sidechain
57	BA	2065	C	Sidechain
57	BA	2068	U	Sidechain
57	BA	207	A	Sidechain
57	BA	2074	U	Sidechain
57	BA	2077	A	Sidechain
57	BA	208	C	Sidechain
57	BA	2080	A	Sidechain
57	BA	2090	A	Sidechain
57	BA	2091	C	Sidechain
57	BA	2097	A	Sidechain
57	BA	21	A	Sidechain
57	BA	2102	G	Sidechain
57	BA	2111	U	Sidechain
57	BA	2112	G	Sidechain
57	BA	2113	U	Sidechain
57	BA	2114	A	Sidechain
57	BA	2120	G	Sidechain
57	BA	2133	G	Sidechain
57	BA	2138	G	Sidechain
57	BA	2152	G	Sidechain
57	BA	2153	C	Sidechain
57	BA	2154	A	Sidechain
57	BA	2167	U	Sidechain
57	BA	2168	G	Sidechain
57	BA	217	A	Sidechain
57	BA	218	A	Sidechain
57	BA	2182	U	Sidechain
57	BA	2188	U	Sidechain
57	BA	219	A	Sidechain
57	BA	2197	U	Sidechain
57	BA	2204	G	Sidechain
57	BA	2205	A	Sidechain

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Mol	Chain	Res	Type	Group
57	BA	2206	C	Sidechain
57	BA	2210	U	Sidechain
57	BA	2226	C	Sidechain
57	BA	2227	A	Sidechain
57	BA	2228	G	Sidechain
57	BA	223	A	Sidechain
57	BA	2230	G	Sidechain
57	BA	2236	U	Sidechain
57	BA	2246	G	Sidechain
57	BA	2252	G	Sidechain
57	BA	2253	G	Sidechain
57	BA	2254	C	Sidechain
57	BA	2258	C	Sidechain
57	BA	226	A	Sidechain
57	BA	2266	A	Sidechain
57	BA	2268	A	Sidechain
57	BA	227	A	Sidechain
57	BA	2273	A	Sidechain
57	BA	2282	G	Sidechain
57	BA	2286	G	Sidechain
57	BA	229	C	Sidechain
57	BA	2295	C	Sidechain
57	BA	2300	C	Sidechain
57	BA	2301	C	Sidechain
57	BA	2304	G	Sidechain
57	BA	2305	U	Sidechain
57	BA	2307	G	Sidechain
57	BA	2308	G	Sidechain
57	BA	231	A	Sidechain
57	BA	2324	U	Sidechain
57	BA	2325	G	Sidechain
57	BA	2327	A	Sidechain
57	BA	2333	A	Sidechain
57	BA	2337	G	Sidechain
57	BA	2341	G	Sidechain
57	BA	2357	G	Sidechain
57	BA	2358	A	Sidechain
57	BA	2365	G	Sidechain
57	BA	2369	A	Sidechain
57	BA	2375	G	Sidechain
57	BA	2376	A	Sidechain
57	BA	2382	G	Sidechain

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Mol	Chain	Res	Type	Group
57	BA	2384	U	Sidechain
57	BA	2391	G	Sidechain
57	BA	2392	A	Sidechain
57	BA	2399	G	Sidechain
57	BA	2400	G	Sidechain
57	BA	2405	G	Sidechain
57	BA	2408	U	Sidechain
57	BA	2411	A	Sidechain
57	BA	2420	C	Sidechain
57	BA	2422	C	Sidechain
57	BA	2424	C	Sidechain
57	BA	243	U	Sidechain
57	BA	2431	U	Sidechain
57	BA	2433	A	Sidechain
57	BA	2437	G	Sidechain
57	BA	2438	U	Sidechain
57	BA	2441	U	Sidechain
57	BA	2442	C	Sidechain
57	BA	2447	G	Sidechain
57	BA	2451	A	Sidechain
57	BA	2453	A	Sidechain
57	BA	2458	G	Sidechain
57	BA	2461	A	Sidechain
57	BA	2468	A	Sidechain
57	BA	2471	A	Sidechain
57	BA	2472	G	Sidechain
57	BA	2475	C	Sidechain
57	BA	2476	A	Sidechain
57	BA	248	G	Sidechain
57	BA	2488	G	Sidechain
57	BA	249	C	Sidechain
57	BA	25	U	Sidechain
57	BA	250	G	Sidechain
57	BA	2507	C	Sidechain
57	BA	2508	G	Sidechain
57	BA	2516	A	Sidechain
57	BA	2517	C	Sidechain
57	BA	2518	A	Sidechain
57	BA	2520	C	Sidechain
57	BA	2521	C	Sidechain
57	BA	2522	U	Sidechain
57	BA	2530	A	Sidechain

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Mol	Chain	Res	Type	Group
57	BA	2531	A	Sidechain
57	BA	2532	G	Sidechain
57	BA	2536	G	Sidechain
57	BA	2542	A	Sidechain
57	BA	2550	G	Sidechain
57	BA	2555	U	Sidechain
57	BA	2557	G	Sidechain
57	BA	2560	A	Sidechain
57	BA	2562	U	Sidechain
57	BA	2565	A	Sidechain
57	BA	2566	A	Sidechain
57	BA	2573	C	Sidechain
57	BA	2575	C	Sidechain
57	BA	2576	G	Sidechain
57	BA	2583	G	Sidechain
57	BA	2588	G	Sidechain
57	BA	2591	C	Sidechain
57	BA	2601	C	Sidechain
57	BA	2608	G	Sidechain
57	BA	2611	C	Sidechain
57	BA	2613	U	Sidechain
57	BA	2624	G	Sidechain
57	BA	2625	G	Sidechain
57	BA	263	G	Sidechain
57	BA	2637	U	Sidechain
57	BA	2638	G	Sidechain
57	BA	264	C	Sidechain
57	BA	2645	G	Sidechain
57	BA	265	A	Sidechain
57	BA	2650	U	Sidechain
57	BA	2659	G	Sidechain
57	BA	2663	G	Sidechain
57	BA	2664	G	Sidechain
57	BA	2679	A	Sidechain
57	BA	2680	U	Sidechain
57	BA	2682	A	Sidechain
57	BA	2700	A	Sidechain
57	BA	2708	G	Sidechain
57	BA	2718	G	Sidechain
57	BA	272	A	Sidechain
57	BA	2721	A	Sidechain
57	BA	2723	C	Sidechain

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Mol	Chain	Res	Type	Group
57	BA	2726	A	Sidechain
57	BA	2727	A	Sidechain
57	BA	2732	G	Sidechain
57	BA	2734	A	Sidechain
57	BA	2737	G	Sidechain
57	BA	2739	U	Sidechain
57	BA	2740	A	Sidechain
57	BA	275	C	Sidechain
57	BA	2751	G	Sidechain
57	BA	2753	A	Sidechain
57	BA	2756	U	Sidechain
57	BA	276	U	Sidechain
57	BA	2768	U	Sidechain
57	BA	277	G	Sidechain
57	BA	2772	C	Sidechain
57	BA	2776	A	Sidechain
57	BA	278	A	Sidechain
57	BA	2780	G	Sidechain
57	BA	2786	U	Sidechain
57	BA	2787	C	Sidechain
57	BA	279	A	Sidechain
57	BA	2796	U	Sidechain
57	BA	2797	U	Sidechain
57	BA	28	A	Sidechain
57	BA	2807	U	Sidechain
57	BA	2809	A	Sidechain
57	BA	2810	A	Sidechain
57	BA	2816	G	Sidechain
57	BA	2824	C	Sidechain
57	BA	2831	G	Sidechain
57	BA	2832	U	Sidechain
57	BA	2836	U	Sidechain
57	BA	2839	G	Sidechain
57	BA	2840	C	Sidechain
57	BA	2848	G	Sidechain
57	BA	2851	A	Sidechain
57	BA	2856	A	Sidechain
57	BA	2857	G	Sidechain
57	BA	2866	U	Sidechain
57	BA	2868	A	Sidechain
57	BA	2869	G	Sidechain
57	BA	2874	C	Sidechain

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Mol	Chain	Res	Type	Group
57	BA	2879	A	Sidechain
57	BA	2881	U	Sidechain
57	BA	2885	G	Sidechain
57	BA	2888	C	Sidechain
57	BA	2889	C	Sidechain
57	BA	2892	G	Sidechain
57	BA	2895	G	Sidechain
57	BA	2899	A	Sidechain
57	BA	293	U	Sidechain
57	BA	297	G	Sidechain
57	BA	301	G	Sidechain
57	BA	303	G	Sidechain
57	BA	307	G	Sidechain
57	BA	308	G	Sidechain
57	BA	313	G	Sidechain
57	BA	33	C	Sidechain
57	BA	333	G	Sidechain
57	BA	343	C	Sidechain
57	BA	346	A	Sidechain
57	BA	347	A	Sidechain
57	BA	352	A	Sidechain
57	BA	354	A	Sidechain
57	BA	361	G	Sidechain
57	BA	363	G	Sidechain
57	BA	367	G	Sidechain
57	BA	374	A	Sidechain
57	BA	377	G	Sidechain
57	BA	380	G	Sidechain
57	BA	385	C	Sidechain
57	BA	39	G	Sidechain
57	BA	390	U	Sidechain
57	BA	392	U	Sidechain
57	BA	394	C	Sidechain
57	BA	395	U	Sidechain
57	BA	403	U	Sidechain
57	BA	415	A	Sidechain
57	BA	416	U	Sidechain
57	BA	418	C	Sidechain
57	BA	420	C	Sidechain
57	BA	422	A	Sidechain
57	BA	43	G	Sidechain
57	BA	442	G	Sidechain

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Mol	Chain	Res	Type	Group
57	BA	446	G	Sidechain
57	BA	447	A	Sidechain
57	BA	449	A	Sidechain
57	BA	45	G	Sidechain
57	BA	450	G	Sidechain
57	BA	455	C	Sidechain
57	BA	457	A	Sidechain
57	BA	459	U	Sidechain
57	BA	460	A	Sidechain
57	BA	461	C	Sidechain
57	BA	463	G	Sidechain
57	BA	464	U	Sidechain
57	BA	474	G	Sidechain
57	BA	477	A	Sidechain
57	BA	478	A	Sidechain
57	BA	48	G	Sidechain
57	BA	480	A	Sidechain
57	BA	481	G	Sidechain
57	BA	486	C	Sidechain
57	BA	492	A	Sidechain
57	BA	493	G	Sidechain
57	BA	498	G	Sidechain
57	BA	500	G	Sidechain
57	BA	501	A	Sidechain
57	BA	507	A	Sidechain
57	BA	510	C	Sidechain
57	BA	52	A	Sidechain
57	BA	528	A	Sidechain
57	BA	53	A	Sidechain
57	BA	544	C	Sidechain
57	BA	568	U	Sidechain
57	BA	573	U	Sidechain
57	BA	575	A	Sidechain
57	BA	576	U	Sidechain
57	BA	577	G	Sidechain
57	BA	58	G	Sidechain
57	BA	581	C	Sidechain
57	BA	583	G	Sidechain
57	BA	587	C	Sidechain
57	BA	59	U	Sidechain
57	BA	592	A	Sidechain
57	BA	594	U	Sidechain

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Mol	Chain	Res	Type	Group
57	BA	60	G	Sidechain
57	BA	603	A	Sidechain
57	BA	607	U	Sidechain
57	BA	608	A	Sidechain
57	BA	611	C	Sidechain
57	BA	617	G	Sidechain
57	BA	622	G	Sidechain
57	BA	623	C	Sidechain
57	BA	626	A	Sidechain
57	BA	63	A	Sidechain
57	BA	630	G	Sidechain
57	BA	632	A	Sidechain
57	BA	636	G	Sidechain
57	BA	637	A	Sidechain
57	BA	642	U	Sidechain
57	BA	666	A	Sidechain
57	BA	671	C	Sidechain
57	BA	672	C	Sidechain
57	BA	676	A	Sidechain
57	BA	685	A	Sidechain
57	BA	687	C	Sidechain
57	BA	688	U	Sidechain
57	BA	692	C	Sidechain
57	BA	693	A	Sidechain
57	BA	697	G	Sidechain
57	BA	700	G	Sidechain
57	BA	708	G	Sidechain
57	BA	71	A	Sidechain
57	BA	715	A	Sidechain
57	BA	717	C	Sidechain
57	BA	718	A	Sidechain
57	BA	72	U	Sidechain
57	BA	721	A	Sidechain
57	BA	726	G	Sidechain
57	BA	728	G	Sidechain
57	BA	729	G	Sidechain
57	BA	73	A	Sidechain
57	BA	735	A	Sidechain
57	BA	736	C	Sidechain
57	BA	738	G	Sidechain
57	BA	74	A	Sidechain
57	BA	75	G	Sidechain

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Mol	Chain	Res	Type	Group
57	BA	751	A	Sidechain
57	BA	757	G	Sidechain
57	BA	764	A	Sidechain
57	BA	772	C	Sidechain
57	BA	776	G	Sidechain
57	BA	78	U	Sidechain
57	BA	782	A	Sidechain
57	BA	783	A	Sidechain
57	BA	786	C	Sidechain
57	BA	789	A	Sidechain
57	BA	791	C	Sidechain
57	BA	794	A	Sidechain
57	BA	795	C	Sidechain
57	BA	800	A	Sidechain
57	BA	801	G	Sidechain
57	BA	802	A	Sidechain
57	BA	804	A	Sidechain
57	BA	810	U	Sidechain
57	BA	813	U	Sidechain
57	BA	819	A	Sidechain
57	BA	820	A	Sidechain
57	BA	828	U	Sidechain
57	BA	834	G	Sidechain
57	BA	837	C	Sidechain
57	BA	838	C	Sidechain
57	BA	841	G	Sidechain
57	BA	845	A	Sidechain
57	BA	858	G	Sidechain
57	BA	86	G	Sidechain
57	BA	861	A	Sidechain
57	BA	867	C	Sidechain
57	BA	87	U	Sidechain
57	BA	871	U	Sidechain
57	BA	876	C	Sidechain
57	BA	881	G	Sidechain
57	BA	883	G	Sidechain
57	BA	89	A	Sidechain
57	BA	894	U	Sidechain
57	BA	902	C	Sidechain
57	BA	905	A	Sidechain
57	BA	909	A	Sidechain
57	BA	910	A	Sidechain

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Mol	Chain	Res	Type	Group
57	BA	912	C	Sidechain
57	BA	914	G	Sidechain
57	BA	915	C	Sidechain
57	BA	916	G	Sidechain
57	BA	923	G	Sidechain
57	BA	927	A	Sidechain
57	BA	931	U	Sidechain
57	BA	934	U	Sidechain
57	BA	936	A	Sidechain
57	BA	940	G	Sidechain
57	BA	945	A	Sidechain
57	BA	950	G	Sidechain
57	BA	956	G	Sidechain
57	BA	957	C	Sidechain
57	BA	959	A	Sidechain
57	BA	962	G	Sidechain
57	BA	963	U	Sidechain
57	BA	966	G	Sidechain
57	BA	968	C	Sidechain
57	BA	969	G	Sidechain
57	BA	970	U	Sidechain
57	BA	971	G	Sidechain
57	BA	983	A	Sidechain
57	BA	984	A	Sidechain
57	BA	989	G	Sidechain
57	BA	99	U	Sidechain
57	BA	990	A	Sidechain
35	BD	155	ARG	Sidechain
55	BH	175	LYS	Peptide
55	BH	57	TYR	Sidechain
26	BJ	137	ARG	Sidechain
28	BN	116	ARG	Sidechain
28	BN	52	ASP	Peptide
29	BO	31	ARG	Sidechain
32	BR	8	ARG	Sidechain
34	BT	71	ARG	Sidechain
36	BU	50	ARG	Sidechain
36	BU	54	ARG	Sidechain
38	BW	25	ARG	Sidechain
40	BY	6	ARG	Sidechain
58	Ba	105	G	Sidechain
58	Ba	11	C	Sidechain

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Mol	Chain	Res	Type	Group
58	Ba	117	G	Sidechain
58	Ba	15	A	Sidechain
58	Ba	21	G	Sidechain
58	Ba	35	C	Sidechain
58	Ba	40	U	Sidechain
58	Ba	41	G	Sidechain
58	Ba	50	A	Sidechain
58	Ba	51	G	Sidechain
58	Ba	57	A	Sidechain
58	Ba	64	G	Sidechain
58	Ba	73	A	Sidechain
58	Ba	90	C	Sidechain
58	Ba	92	C	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AJ	794	0	803	0	0
2	AK	923	0	912	0	0
3	AL	923	0	954	0	0
4	AM	876	0	910	0	0
5	AN	771	0	777	0	0
6	AO	690	0	691	0	0
7	AP	620	0	611	0	0
8	AQ	657	0	687	0	0
9	AR	603	0	602	0	0
10	AS	708	0	732	0	0
11	AB	1805	0	1750	0	0
12	AT	636	0	652	0	0
13	AU	564	0	579	0	0
14	AC	1761	0	1793	0	0
15	AD	1587	0	1596	0	0
16	AE	1182	0	1185	0	0
17	AF	1061	0	971	0	0
18	AG	1347	0	1347	0	0
19	AH	948	0	975	0	0
20	AI	1000	0	1011	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	A1	4989	0	4915	0	0
22	AA	33089	0	16668	0	0
23	A2	993	0	501	0	0
24	A3	1640	0	845	0	0
25	BC	1733	0	1824	0	0
26	BJ	1233	0	1283	0	0
27	BK	1032	0	1088	0	0
28	BN	1129	0	1162	0	0
29	BO	947	0	1023	0	0
30	BP	1053	0	1129	0	0
31	BQ	1074	0	1157	0	0
32	BR	1008	0	1045	0	0
33	BS	900	0	935	0	0
34	BT	917	0	965	0	0
35	BD	2092	0	2170	0	0
36	BU	947	0	1022	0	0
37	BV	816	0	839	0	0
38	BW	857	0	922	0	0
39	BX	787	0	846	0	0
40	BY	789	0	847	0	0
41	BZ	753	0	780	0	0
42	B0	634	0	656	0	0
43	B1	625	0	655	0	0
44	B2	509	0	543	0	0
45	BE	1565	0	1616	0	0
46	B3	449	0	491	0	0
47	B4	549	0	552	0	0
48	B5	444	0	461	0	0
49	B6	441	0	485	0	0
50	B7	377	0	418	0	0
51	B8	504	0	574	0	0
52	B9	302	0	343	0	0
53	BF	1552	0	1619	0	0
54	BG	1420	0	1460	0	0
55	BH	1323	0	1374	0	0
56	BL	1111	0	1148	0	0
57	BA	62351	0	31378	0	0
58	Ba	2566	0	1302	0	0
All	All	154956	0	106579	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AJ	44/103 (43%)	40 (91%)	1 (2%)	3 (7%)	1	11
2	AK	57/128 (44%)	52 (91%)	5 (9%)	0	100	100
3	AL	64/123 (52%)	54 (84%)	8 (12%)	2 (3%)	3	22
4	AM	56/117 (48%)	51 (91%)	4 (7%)	1 (2%)	6	34
5	AN	41/100 (41%)	37 (90%)	3 (7%)	1 (2%)	4	27
6	AO	44/88 (50%)	43 (98%)	1 (2%)	0	100	100
7	AP	34/82 (42%)	31 (91%)	3 (9%)	0	100	100
8	AQ	52/83 (63%)	48 (92%)	4 (8%)	0	100	100
9	AR	36/74 (49%)	34 (94%)	2 (6%)	0	100	100
10	AS	54/91 (59%)	53 (98%)	1 (2%)	0	100	100
11	AB	123/240 (51%)	114 (93%)	7 (6%)	2 (2%)	7	38
12	AT	32/86 (37%)	30 (94%)	2 (6%)	0	100	100
13	AU	24/70 (34%)	18 (75%)	3 (12%)	3 (12%)	0	4
14	AC	126/232 (54%)	122 (97%)	4 (3%)	0	100	100
15	AD	107/205 (52%)	102 (95%)	5 (5%)	0	100	100
16	AE	89/166 (54%)	84 (94%)	4 (4%)	1 (1%)	11	46
17	AF	65/135 (48%)	61 (94%)	4 (6%)	0	100	100
18	AG	84/178 (47%)	79 (94%)	5 (6%)	0	100	100
19	AH	77/129 (60%)	70 (91%)	7 (9%)	0	100	100
20	AI	69/129 (54%)	63 (91%)	6 (9%)	0	100	100
21	A1	434/639 (68%)	390 (90%)	38 (9%)	6 (1%)	9	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	BC	232/234 (99%)	213 (92%)	18 (8%)	1 (0%)	30	67
26	BJ	162/164 (99%)	158 (98%)	3 (2%)	1 (1%)	21	59
27	BK	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
28	BN	140/142 (99%)	131 (94%)	9 (6%)	0	100	100
29	BO	121/123 (98%)	107 (88%)	11 (9%)	3 (2%)	4	26
30	BP	142/144 (99%)	127 (89%)	13 (9%)	2 (1%)	9	40
31	BQ	134/136 (98%)	126 (94%)	6 (4%)	2 (2%)	8	40
32	BR	125/127 (98%)	112 (90%)	11 (9%)	2 (2%)	7	38
33	BS	115/117 (98%)	115 (100%)	0	0	100	100
34	BT	112/114 (98%)	107 (96%)	3 (3%)	2 (2%)	6	34
35	BD	270/272 (99%)	252 (93%)	15 (6%)	3 (1%)	11	46
36	BU	115/117 (98%)	108 (94%)	5 (4%)	2 (2%)	7	36
37	BV	101/103 (98%)	94 (93%)	4 (4%)	3 (3%)	3	23
38	BW	108/110 (98%)	103 (95%)	4 (4%)	1 (1%)	14	51
39	BX	98/100 (98%)	83 (85%)	12 (12%)	3 (3%)	3	22
40	BY	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
41	BZ	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
42	B0	82/84 (98%)	72 (88%)	6 (7%)	4 (5%)	1	16
43	B1	75/77 (97%)	69 (92%)	5 (7%)	1 (1%)	9	42
44	B2	61/63 (97%)	54 (88%)	7 (12%)	0	100	100
45	BE	207/209 (99%)	181 (87%)	20 (10%)	6 (3%)	3	23
46	B3	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
47	B4	68/70 (97%)	62 (91%)	6 (9%)	0	100	100
48	B5	54/56 (96%)	50 (93%)	3 (6%)	1 (2%)	6	32
49	B6	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
50	B7	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
51	B8	62/64 (97%)	61 (98%)	1 (2%)	0	100	100
52	B9	36/38 (95%)	31 (86%)	3 (8%)	2 (6%)	1	14
53	BF	199/201 (99%)	186 (94%)	7 (4%)	6 (3%)	3	23
54	BG	176/178 (99%)	155 (88%)	15 (8%)	6 (3%)	3	21
55	BH	174/176 (99%)	157 (90%)	14 (8%)	3 (2%)	7	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
56	BL	147/149 (99%)	133 (90%)	13 (9%)	1 (1%)	18	56
All	All	5512/7062 (78%)	5089 (92%)	349 (6%)	74 (1%)	12	42

All (74) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	A1	242	THR
21	A1	493	LYS
32	BR	13	ASN
35	BD	140	VAL
42	B0	40	ARG
45	BE	122	VAL
56	BL	35	LYS
1	AJ	57	VAL
13	AU	3	ILE
13	AU	19	LYS
21	A1	174	GLN
30	BP	53	GLY
34	BT	5	LYS
35	BD	77	VAL
42	B0	36	ILE
43	B1	27	ARG
45	BE	37	VAL
53	BF	62	GLN
53	BF	79	ARG
53	BF	96	VAL
54	BG	132	ARG
55	BH	29	ASN
55	BH	46	ASP
4	AM	22	TYR
11	AB	18	GLN
16	AE	23	THR
21	A1	249	LEU
21	A1	284	SER
21	A1	566	VAL
30	BP	36	LYS
31	BQ	43	ALA
36	BU	5	ARG
38	BW	28	LYS
39	BX	51	PHE
53	BF	6	LYS
53	BF	46	GLN

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Mol	Chain	Res	Type
54	BG	80	GLN
3	AL	75	GLU
31	BQ	58	LYS
35	BD	162	GLN
36	BU	102	LYS
37	BV	91	GLN
39	BX	69	ARG
42	B0	23	LYS
52	B9	16	ILE
1	AJ	42	LEU
3	AL	43	LYS
11	AB	17	HIS
25	BC	166	ASP
26	BJ	70	CYS
37	BV	53	PHE
42	B0	68	PHE
45	BE	119	ALA
45	BE	167	ASN
54	BG	81	GLY
54	BG	88	VAL
54	BG	103	ILE
55	BH	94	ARG
29	BO	5	GLN
32	BR	80	PHE
37	BV	101	ILE
39	BX	74	ILE
45	BE	113	SER
48	B5	54	ILE
53	BF	183	PHE
54	BG	35	LEU
1	AJ	74	VAL
34	BT	32	VAL
45	BE	117	GLY
52	B9	7	VAL
29	BO	93	GLN
29	BO	122	VAL
5	AN	71	GLY
13	AU	2	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AJ	90/90 (100%)	88 (98%)	2 (2%)	45	64
2	AK	98/98 (100%)	96 (98%)	2 (2%)	48	66
3	AL	103/103 (100%)	102 (99%)	1 (1%)	68	78
4	AM	95/95 (100%)	95 (100%)	0	100	100
5	AN	83/83 (100%)	82 (99%)	1 (1%)	63	75
6	AO	76/76 (100%)	75 (99%)	1 (1%)	61	74
7	AP	65/65 (100%)	64 (98%)	1 (2%)	57	72
8	AQ	77/77 (100%)	77 (100%)	0	100	100
9	AR	64/64 (100%)	62 (97%)	2 (3%)	35	56
10	AS	78/78 (100%)	75 (96%)	3 (4%)	29	50
11	AB	198/198 (100%)	197 (100%)	1 (0%)	81	83
12	AT	65/65 (100%)	65 (100%)	0	100	100
13	AU	60/60 (100%)	58 (97%)	2 (3%)	33	55
14	AC	189/189 (100%)	184 (97%)	5 (3%)	40	62
15	AD	172/172 (100%)	170 (99%)	2 (1%)	63	75
16	AE	125/125 (100%)	119 (95%)	6 (5%)	23	44
17	AF	116/116 (100%)	112 (97%)	4 (3%)	32	54
18	AG	146/146 (100%)	144 (99%)	2 (1%)	59	72
19	AH	104/104 (100%)	104 (100%)	0	100	100
20	AI	106/106 (100%)	105 (99%)	1 (1%)	70	79
21	A1	568/568 (100%)	559 (98%)	9 (2%)	55	70
25	BC	181/181 (100%)	177 (98%)	4 (2%)	45	64
26	BJ	122/122 (100%)	120 (98%)	2 (2%)	55	70
27	BK	109/109 (100%)	106 (97%)	3 (3%)	38	60
28	BN	116/116 (100%)	111 (96%)	5 (4%)	26	47
29	BO	104/104 (100%)	101 (97%)	3 (3%)	37	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	BP	103/103 (100%)	99 (96%)	4 (4%)	28	49
31	BQ	109/109 (100%)	105 (96%)	4 (4%)	30	51
32	BR	103/103 (100%)	100 (97%)	3 (3%)	37	58
33	BS	87/87 (100%)	86 (99%)	1 (1%)	65	76
34	BT	99/99 (100%)	98 (99%)	1 (1%)	68	78
35	BD	217/217 (100%)	214 (99%)	3 (1%)	59	72
36	BU	89/89 (100%)	86 (97%)	3 (3%)	32	54
37	BV	84/84 (100%)	83 (99%)	1 (1%)	63	75
38	BW	93/93 (100%)	91 (98%)	2 (2%)	45	64
39	BX	84/84 (100%)	83 (99%)	1 (1%)	63	75
40	BY	84/84 (100%)	83 (99%)	1 (1%)	63	75
41	BZ	78/78 (100%)	77 (99%)	1 (1%)	61	74
42	B0	62/62 (100%)	56 (90%)	6 (10%)	8	24
43	B1	67/67 (100%)	67 (100%)	0	100	100
44	B2	55/55 (100%)	55 (100%)	0	100	100
45	BE	164/164 (100%)	162 (99%)	2 (1%)	63	75
46	B3	48/48 (100%)	48 (100%)	0	100	100
47	B4	62/62 (100%)	61 (98%)	1 (2%)	55	70
48	B5	47/47 (100%)	45 (96%)	2 (4%)	26	47
49	B6	48/48 (100%)	48 (100%)	0	100	100
50	B7	38/38 (100%)	38 (100%)	0	100	100
51	B8	51/51 (100%)	50 (98%)	1 (2%)	48	66
52	B9	34/34 (100%)	34 (100%)	0	100	100
53	BF	165/165 (100%)	163 (99%)	2 (1%)	63	75
54	BG	149/149 (100%)	145 (97%)	4 (3%)	39	61
55	BH	137/137 (100%)	134 (98%)	3 (2%)	45	64
56	BL	114/114 (100%)	114 (100%)	0	100	100
All	All	5781/5781 (100%)	5673 (98%)	108 (2%)	49	67

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AJ	58	ASN

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Mol	Chain	Res	Type
1	AJ	59	LYS
2	AK	5	ILE
2	AK	55	ARG
3	AL	49	ARG
5	AN	95	LEU
6	AO	88	ARG
7	AP	47	GLU
9	AR	15	GLU
9	AR	65	SER
10	AS	82	HIS
10	AS	86	LYS
10	AS	91	LYS
11	AB	183	PHE
13	AU	19	LYS
13	AU	68	ARG
14	AC	35	ASP
14	AC	48	LYS
14	AC	57	GLU
14	AC	187	GLU
14	AC	227	GLN
15	AD	131	ILE
15	AD	187	ARG
16	AE	12	GLU
16	AE	22	LYS
16	AE	49	TYR
16	AE	92	ARG
16	AE	121	ASN
16	AE	122	VAL
17	AF	6	ILE
17	AF	69	GLU
17	AF	98	GLU
17	AF	118	ASN
18	AG	143	MET
18	AG	150	PHE
20	AI	79	ARG
21	A1	228	ARG
21	A1	256	ILE
21	A1	322	GLN
21	A1	370	ASP
21	A1	421	MET
21	A1	468	TYR
21	A1	490	TYR

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Mol	Chain	Res	Type
21	A1	526	GLN
21	A1	561	TYR
25	BC	39	VAL
25	BC	162	ARG
25	BC	208	TYR
25	BC	234	ASN
26	BJ	55	ARG
26	BJ	94	LEU
27	BK	4	VAL
27	BK	45	THR
27	BK	87	SER
28	BN	2	LYS
28	BN	44	TYR
28	BN	47	HIS
28	BN	61	LYS
28	BN	98	GLU
29	BO	47	ILE
29	BO	107	LEU
29	BO	122	VAL
30	BP	4	ASN
30	BP	21	ARG
30	BP	39	LYS
30	BP	111	ILE
31	BQ	12	MET
31	BQ	63	ILE
31	BQ	93	VAL
31	BQ	97	GLN
32	BR	1	MET
32	BR	16	HIS
32	BR	99	LYS
33	BS	18	LEU
34	BT	109	ILE
35	BD	211	ARG
35	BD	212	TRP
35	BD	217	PRO
36	BU	4	LYS
36	BU	88	GLU
36	BU	96	ASP
37	BV	49	ILE
38	BW	60	HIS
38	BW	95	ARG
39	BX	76	ARG

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Mol	Chain	Res	Type
40	BY	71	ILE
41	BZ	71	LYS
42	B0	22	VAL
42	B0	23	LYS
42	B0	35	ILE
42	B0	40	ARG
42	B0	49	ASN
42	B0	70	VAL
45	BE	29	VAL
45	BE	128	ARG
47	B4	63	ARG
48	B5	6	LYS
48	B5	32	THR
51	B8	57	VAL
53	BF	67	ARG
53	BF	88	ARG
54	BG	34	THR
54	BG	94	ARG
54	BG	103	ILE
54	BG	111	ARG
55	BH	2	ARG
55	BH	154	GLU
55	BH	166	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
22	AA	1541/1542 (99%)	204 (13%)	57 (3%)
23	A2	46/47 (97%)	13 (28%)	1 (2%)
24	A3	75/77 (97%)	12 (16%)	2 (2%)
57	BA	2903/2904 (99%)	434 (14%)	115 (3%)
58	Ba	119/120 (99%)	14 (11%)	0
All	All	4684/4690 (99%)	677 (14%)	175 (3%)

All (677) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
22	AA	2	A

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Mol	Chain	Res	Type
22	AA	3	A
22	AA	5	U
22	AA	6	G
22	AA	7	A
22	AA	8	A
22	AA	9	G
22	AA	32	A
22	AA	39	G
22	AA	48	C
22	AA	49	U
22	AA	50	A
22	AA	52	C
22	AA	55	A
22	AA	56	U
22	AA	60	A
22	AA	84	U
22	AA	108	G
22	AA	109	A
22	AA	120	A
22	AA	131	A
22	AA	144	G
22	AA	149	A
22	AA	153	C
22	AA	163	C
22	AA	184	G
22	AA	204	G
22	AA	205	A
22	AA	206	C
22	AA	214	C
22	AA	243	A
22	AA	244	U
22	AA	247	G
22	AA	250	A
22	AA	251	G
22	AA	262	A
22	AA	263	A
22	AA	266	G
22	AA	267	C
22	AA	280	C
22	AA	289	G
22	AA	298	A
22	AA	328	C

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Mol	Chain	Res	Type
22	AA	329	A
22	AA	330	C
22	AA	332	G
22	AA	347	G
22	AA	352	C
22	AA	353	A
22	AA	354	G
22	AA	367	U
22	AA	368	U
22	AA	372	C
22	AA	373	A
22	AA	381	C
22	AA	390	U
22	AA	398	U
22	AA	406	G
22	AA	412	A
22	AA	413	G
22	AA	422	C
22	AA	429	U
22	AA	451	A
22	AA	464	U
22	AA	465	A
22	AA	466	A
22	AA	468	A
22	AA	481	G
22	AA	482	A
22	AA	484	G
22	AA	486	U
22	AA	487	A
22	AA	494	G
22	AA	496	A
22	AA	498	A
22	AA	505	G
22	AA	508	U
22	AA	511	C
22	AA	512	U
22	AA	518	C
22	AA	519	C
22	AA	520	A
22	AA	524	G
22	AA	527	7MG
22	AA	531	U

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Mol	Chain	Res	Type
22	AA	532	A
22	AA	547	A
22	AA	559	A
22	AA	564	C
22	AA	566	G
22	AA	572	A
22	AA	573	A
22	AA	576	C
22	AA	631	C
22	AA	633	G
22	AA	665	A
22	AA	688	G
22	AA	695	A
22	AA	718	A
22	AA	719	C
22	AA	720	C
22	AA	721	G
22	AA	723	U
22	AA	755	G
22	AA	765	G
22	AA	766	A
22	AA	812	G
22	AA	813	U
22	AA	817	C
22	AA	821	G
22	AA	828	U
22	AA	840	C
22	AA	841	C
22	AA	843	U
22	AA	846	G
22	AA	874	G
22	AA	885	G
22	AA	889	A
22	AA	890	G
22	AA	914	A
22	AA	927	G
22	AA	934	C
22	AA	935	A
22	AA	938	A
22	AA	960	U
22	AA	962	C
22	AA	966	2MG

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Mol	Chain	Res	Type
22	AA	968	A
22	AA	969	A
22	AA	975	A
22	AA	977	A
22	AA	981	U
22	AA	993	G
22	AA	1004	A
22	AA	1026	G
22	AA	1044	A
22	AA	1050	G
22	AA	1051	C
22	AA	1064	G
22	AA	1065	U
22	AA	1094	G
22	AA	1101	A
22	AA	1102	A
22	AA	1110	A
22	AA	1136	C
22	AA	1138	G
22	AA	1139	G
22	AA	1140	C
22	AA	1152	A
22	AA	1159	U
22	AA	1168	U
22	AA	1169	A
22	AA	1183	U
22	AA	1184	G
22	AA	1191	A
22	AA	1196	A
22	AA	1212	U
22	AA	1214	C
22	AA	1215	G
22	AA	1225	A
22	AA	1226	C
22	AA	1228	C
22	AA	1238	A
22	AA	1239	A
22	AA	1241	G
22	AA	1256	A
22	AA	1257	A
22	AA	1258	G
22	AA	1279	G

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Mol	Chain	Res	Type
22	AA	1280	A
22	AA	1281	C
22	AA	1282	C
22	AA	1285	A
22	AA	1297	G
22	AA	1302	C
22	AA	1303	C
22	AA	1305	G
22	AA	1306	A
22	AA	1319	A
22	AA	1320	C
22	AA	1322	C
22	AA	1340	A
22	AA	1346	A
22	AA	1359	C
22	AA	1360	A
22	AA	1398	A
22	AA	1401	G
22	AA	1447	A
22	AA	1491	G
22	AA	1492	A
22	AA	1493	A
22	AA	1502	A
22	AA	1503	A
22	AA	1506	U
22	AA	1507	A
22	AA	1520	C
22	AA	1529	G
22	AA	1530	G
22	AA	1535	C
22	AA	1537	U
22	AA	1538	C
22	AA	1539	C
22	AA	1540	U
22	AA	1542	A
23	A2	14	G
23	A2	16	A
23	A2	19	A
23	A2	21	U
23	A2	25	U
23	A2	26	U
23	A2	27	A

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Mol	Chain	Res	Type
23	A2	29	G
23	A2	30	U
23	A2	34	U
23	A2	46	C
23	A2	47	C
23	A2	56	G
24	A3	2	G
24	A3	9	G
24	A3	10	G
24	A3	16	C
24	A3	17	C
24	A3	21	H2U
24	A3	39	A
24	A3	49	C
24	A3	74	A
24	A3	75	C
24	A3	76	C
24	A3	77	A
57	BA	13	A
57	BA	35	G
57	BA	61	C
57	BA	62	U
57	BA	71	A
57	BA	74	A
57	BA	75	G
57	BA	91	A
57	BA	98	G
57	BA	100	U
57	BA	119	A
57	BA	120	U
57	BA	139	U
57	BA	140	C
57	BA	149	A
57	BA	163	C
57	BA	180	G
57	BA	196	A
57	BA	197	A
57	BA	199	A
57	BA	204	A
57	BA	205	G
57	BA	216	A
57	BA	222	A

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Mol	Chain	Res	Type
57	BA	230	G
57	BA	242	G
57	BA	243	U
57	BA	248	G
57	BA	250	G
57	BA	265	A
57	BA	266	G
57	BA	271	G
57	BA	272	A
57	BA	277	G
57	BA	299	A
57	BA	311	A
57	BA	312	G
57	BA	324	A
57	BA	330	A
57	BA	332	A
57	BA	333	G
57	BA	338	G
57	BA	360	U
57	BA	361	G
57	BA	368	A
57	BA	372	G
57	BA	386	G
57	BA	387	U
57	BA	388	G
57	BA	394	C
57	BA	395	U
57	BA	396	G
57	BA	406	G
57	BA	411	G
57	BA	424	G
57	BA	435	C
57	BA	451	U
57	BA	454	A
57	BA	458	G
57	BA	479	A
57	BA	480	A
57	BA	481	G
57	BA	482	A
57	BA	489	G
57	BA	490	C
57	BA	491	G

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Mol	Chain	Res	Type
57	BA	504	A
57	BA	505	A
57	BA	531	C
57	BA	532	A
57	BA	533	G
57	BA	544	C
57	BA	545	U
57	BA	546	U
57	BA	550	C
57	BA	562	U
57	BA	573	U
57	BA	575	A
57	BA	588	U
57	BA	603	A
57	BA	604	G
57	BA	613	A
57	BA	615	U
57	BA	637	A
57	BA	638	G
57	BA	652	U
57	BA	654	A
57	BA	671	C
57	BA	686	U
57	BA	718	A
57	BA	719	C
57	BA	730	A
57	BA	747	5MU
57	BA	752	A
57	BA	753	A
57	BA	764	A
57	BA	776	G
57	BA	781	A
57	BA	782	A
57	BA	783	A
57	BA	784	G
57	BA	789	A
57	BA	790	U
57	BA	791	C
57	BA	792	A
57	BA	805	G
57	BA	812	C
57	BA	846	U

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Mol	Chain	Res	Type
57	BA	850	U
57	BA	851	C
57	BA	859	G
57	BA	866	A
57	BA	867	C
57	BA	887	U
57	BA	890	C
57	BA	896	A
57	BA	901	C
57	BA	910	A
57	BA	914	G
57	BA	915	C
57	BA	920	A
57	BA	921	C
57	BA	945	A
57	BA	946	C
57	BA	961	C
57	BA	974	G
57	BA	995	C
57	BA	996	A
57	BA	1009	A
57	BA	1012	U
57	BA	1019	U
57	BA	1020	A
57	BA	1022	G
57	BA	1025	G
57	BA	1033	U
57	BA	1034	G
57	BA	1046	A
57	BA	1047	G
57	BA	1048	A
57	BA	1057	A
57	BA	1062	G
57	BA	1065	U
57	BA	1066	U
57	BA	1068	G
57	BA	1069	A
57	BA	1070	A
57	BA	1071	G
57	BA	1073	A
57	BA	1078	U
57	BA	1079	C

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Mol	Chain	Res	Type
57	BA	1087	G
57	BA	1088	A
57	BA	1095	A
57	BA	1096	A
57	BA	1098	A
57	BA	1112	G
57	BA	1128	G
57	BA	1129	A
57	BA	1130	U
57	BA	1132	U
57	BA	1133	A
57	BA	1135	C
57	BA	1143	A
57	BA	1155	A
57	BA	1175	A
57	BA	1176	U
57	BA	1177	G
57	BA	1212	G
57	BA	1225	G
57	BA	1238	G
57	BA	1241	A
57	BA	1248	G
57	BA	1254	A
57	BA	1255	U
57	BA	1256	G
57	BA	1257	C
57	BA	1266	G
57	BA	1271	G
57	BA	1272	A
57	BA	1273	U
57	BA	1286	A
57	BA	1287	A
57	BA	1300	G
57	BA	1301	A
57	BA	1302	A
57	BA	1303	G
57	BA	1313	U
57	BA	1314	C
57	BA	1324	G
57	BA	1325	U
57	BA	1329	U
57	BA	1332	G

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Mol	Chain	Res	Type
57	BA	1333	G
57	BA	1341	G
57	BA	1348	C
57	BA	1349	C
57	BA	1350	C
57	BA	1365	A
57	BA	1366	A
57	BA	1379	U
57	BA	1383	A
57	BA	1384	A
57	BA	1386	C
57	BA	1394	U
57	BA	1396	U
57	BA	1416	G
57	BA	1417	C
57	BA	1451	C
57	BA	1452	G
57	BA	1455	G
57	BA	1458	U
57	BA	1459	G
57	BA	1475	G
57	BA	1482	G
57	BA	1493	C
57	BA	1508	A
57	BA	1509	A
57	BA	1524	G
57	BA	1552	A
57	BA	1568	G
57	BA	1569	A
57	BA	1598	A
57	BA	1607	C
57	BA	1608	A
57	BA	1610	A
57	BA	1611	C
57	BA	1614	A
57	BA	1615	C
57	BA	1646	C
57	BA	1647	U
57	BA	1648	U
57	BA	1654	A
57	BA	1668	A
57	BA	1669	A

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Mol	Chain	Res	Type
57	BA	1674	G
57	BA	1675	C
57	BA	1700	A
57	BA	1713	A
57	BA	1729	U
57	BA	1730	C
57	BA	1732	C
57	BA	1733	G
57	BA	1758	U
57	BA	1762	A
57	BA	1764	C
57	BA	1773	A
57	BA	1786	A
57	BA	1787	A
57	BA	1791	A
57	BA	1800	C
57	BA	1816	C
57	BA	1839	G
57	BA	1900	A
57	BA	1901	A
57	BA	1906	G
57	BA	1912	A
57	BA	1914	C
57	BA	1919	A
57	BA	1928	A
57	BA	1929	G
57	BA	1930	G
57	BA	1937	A
57	BA	1941	C
57	BA	1942	C
57	BA	1955	U
57	BA	1964	G
57	BA	1965	C
57	BA	1966	A
57	BA	1970	A
57	BA	1971	U
57	BA	1972	G
57	BA	1982	U
57	BA	1992	G
57	BA	1993	U
57	BA	1998	A
57	BA	2023	C

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Mol	Chain	Res	Type
57	BA	2031	A
57	BA	2032	G
57	BA	2042	A
57	BA	2043	C
57	BA	2056	G
57	BA	2060	A
57	BA	2061	G
57	BA	2062	A
57	BA	2063	C
57	BA	2068	U
57	BA	2069	7MG
57	BA	2076	U
57	BA	2077	A
57	BA	2092	U
57	BA	2093	G
57	BA	2111	U
57	BA	2112	G
57	BA	2113	U
57	BA	2116	G
57	BA	2117	A
57	BA	2118	U
57	BA	2119	A
57	BA	2126	A
57	BA	2127	G
57	BA	2130	U
57	BA	2131	U
57	BA	2132	U
57	BA	2133	G
57	BA	2134	A
57	BA	2146	C
57	BA	2147	A
57	BA	2148	G
57	BA	2154	A
57	BA	2158	A
57	BA	2164	C
57	BA	2165	C
57	BA	2170	A
57	BA	2198	A
57	BA	2203	U
57	BA	2212	A
57	BA	2213	U
57	BA	2239	G

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Mol	Chain	Res	Type
57	BA	2249	U
57	BA	2250	G
57	BA	2251	OMG
57	BA	2253	G
57	BA	2254	C
57	BA	2266	A
57	BA	2276	G
57	BA	2282	G
57	BA	2283	C
57	BA	2287	A
57	BA	2288	A
57	BA	2289	G
57	BA	2306	C
57	BA	2307	G
57	BA	2308	G
57	BA	2309	A
57	BA	2312	U
57	BA	2321	U
57	BA	2325	G
57	BA	2327	A
57	BA	2333	A
57	BA	2334	U
57	BA	2335	A
57	BA	2336	A
57	BA	2337	G
57	BA	2345	G
57	BA	2346	A
57	BA	2347	C
57	BA	2382	G
57	BA	2383	G
57	BA	2385	C
57	BA	2390	U
57	BA	2402	U
57	BA	2403	C
57	BA	2423	U
57	BA	2424	C
57	BA	2425	A
57	BA	2426	A
57	BA	2428	G
57	BA	2429	G
57	BA	2430	A
57	BA	2431	U

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Mol	Chain	Res	Type
57	BA	2433	A
57	BA	2435	A
57	BA	2439	A
57	BA	2441	U
57	BA	2447	G
57	BA	2448	A
57	BA	2449	H2U
57	BA	2452	C
57	BA	2472	G
57	BA	2476	A
57	BA	2478	A
57	BA	2489	U
57	BA	2490	G
57	BA	2491	U
57	BA	2492	U
57	BA	2493	U
57	BA	2501	C
57	BA	2502	G
57	BA	2504	PSU
57	BA	2505	G
57	BA	2507	C
57	BA	2513	A
57	BA	2518	A
57	BA	2519	U
57	BA	2529	G
57	BA	2530	A
57	BA	2534	A
57	BA	2555	U
57	BA	2564	A
57	BA	2565	A
57	BA	2566	A
57	BA	2572	A
57	BA	2573	C
57	BA	2574	G
57	BA	2577	A
57	BA	2585	U
57	BA	2599	G
57	BA	2602	A
57	BA	2613	U
57	BA	2615	U
57	BA	2616	C
57	BA	2629	U

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Mol	Chain	Res	Type
57	BA	2654	A
57	BA	2655	G
57	BA	2656	U
57	BA	2658	C
57	BA	2659	G
57	BA	2660	A
57	BA	2661	G
57	BA	2663	G
57	BA	2685	G
57	BA	2689	U
57	BA	2690	U
57	BA	2714	G
57	BA	2733	A
57	BA	2755	C
57	BA	2756	U
57	BA	2757	A
57	BA	2778	A
57	BA	2790	U
57	BA	2791	G
57	BA	2792	A
57	BA	2797	U
57	BA	2799	A
57	BA	2800	A
57	BA	2820	A
57	BA	2823	A
57	BA	2834	G
57	BA	2850	A
57	BA	2886	A
57	BA	2894	G
57	BA	2895	G
57	BA	2903	U
57	BA	2904	U
58	Ba	12	C
58	Ba	13	G
58	Ba	14	U
58	Ba	15	A
58	Ba	16	G
58	Ba	25	U
58	Ba	41	G
58	Ba	42	C
58	Ba	88	C
58	Ba	89	U

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Mol	Chain	Res	Type
58	Ba	90	C
58	Ba	99	A
58	Ba	109	A
58	Ba	120	U

All (175) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	AA	2	A
22	AA	3	A
22	AA	5	U
22	AA	6	G
22	AA	13	U
22	AA	48	C
22	AA	49	U
22	AA	51	A
22	AA	71	A
22	AA	121	U
22	AA	161	A
22	AA	197	A
22	AA	205	A
22	AA	243	A
22	AA	262	A
22	AA	279	A
22	AA	297	G
22	AA	305	G
22	AA	328	C
22	AA	329	A
22	AA	331	G
22	AA	367	U
22	AA	372	C
22	AA	412	A
22	AA	451	A
22	AA	464	U
22	AA	465	A
22	AA	497	G
22	AA	531	U
22	AA	575	G
22	AA	619	U
22	AA	700	G
22	AA	717	U
22	AA	719	C

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Mol	Chain	Res	Type
22	AA	765	G
22	AA	812	G
22	AA	840	C
22	AA	845	A
22	AA	934	C
22	AA	974	A
22	AA	1101	A
22	AA	1183	U
22	AA	1213	A
22	AA	1214	C
22	AA	1225	A
22	AA	1238	A
22	AA	1256	A
22	AA	1281	C
22	AA	1302	C
22	AA	1305	G
22	AA	1319	A
22	AA	1380	U
22	AA	1397	C
22	AA	1491	G
22	AA	1529	G
22	AA	1537	U
22	AA	1539	C
23	A2	33	A
24	A3	9	G
24	A3	10	G
57	BA	13	A
57	BA	48	G
57	BA	61	C
57	BA	119	A
57	BA	121	G
57	BA	140	C
57	BA	190	A
57	BA	196	A
57	BA	242	G
57	BA	249	C
57	BA	301	G
57	BA	311	A
57	BA	332	A
57	BA	387	U
57	BA	394	C
57	BA	395	U

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Mol	Chain	Res	Type
57	BA	479	A
57	BA	489	G
57	BA	529	A
57	BA	544	C
57	BA	545	U
57	BA	561	G
57	BA	587	C
57	BA	603	A
57	BA	620	G
57	BA	637	A
57	BA	651	G
57	BA	653	U
57	BA	718	A
57	BA	752	A
57	BA	782	A
57	BA	804	A
57	BA	850	U
57	BA	859	G
57	BA	866	A
57	BA	896	A
57	BA	920	A
57	BA	958	U
57	BA	960	A
57	BA	995	C
57	BA	1019	U
57	BA	1033	U
57	BA	1061	U
57	BA	1078	U
57	BA	1088	A
57	BA	1095	A
57	BA	1128	G
57	BA	1133	A
57	BA	1142	A
57	BA	1254	A
57	BA	1256	G
57	BA	1286	A
57	BA	1301	A
57	BA	1313	U
57	BA	1324	G
57	BA	1325	U
57	BA	1332	G
57	BA	1349	C

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Mol	Chain	Res	Type
57	BA	1365	A
57	BA	1393	A
57	BA	1451	C
57	BA	1458	U
57	BA	1474	U
57	BA	1508	A
57	BA	1568	G
57	BA	1607	C
57	BA	1610	A
57	BA	1614	A
57	BA	1646	C
57	BA	1647	U
57	BA	1653	G
57	BA	1668	A
57	BA	1674	G
57	BA	1729	U
57	BA	1758	U
57	BA	1786	A
57	BA	1929	G
57	BA	1937	A
57	BA	1939	5MU
57	BA	1941	C
57	BA	2042	A
57	BA	2060	A
57	BA	2061	G
57	BA	2062	A
57	BA	2068	U
57	BA	2076	U
57	BA	2092	U
57	BA	2117	A
57	BA	2131	U
57	BA	2133	G
57	BA	2248	C
57	BA	2251	OMG
57	BA	2253	G
57	BA	2308	G
57	BA	2336	A
57	BA	2345	G
57	BA	2402	U
57	BA	2422	C
57	BA	2423	U
57	BA	2430	A

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Mol	Chain	Res	Type
57	BA	2440	C
57	BA	2447	G
57	BA	2489	U
57	BA	2529	G
57	BA	2564	A
57	BA	2571	U
57	BA	2615	U
57	BA	2629	U
57	BA	2655	G
57	BA	2660	A
57	BA	2755	C
57	BA	2756	U
57	BA	2790	U
57	BA	2885	G
57	BA	2894	G

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

39 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	$\# Z > 2$
57	3TD	BA	1915	57	19,22,23	0.81	0	23,32,35	1.44	3 (13%)
57	OMC	BA	2498	57	19,22,23	0.75	0	25,31,34	1.29	1 (4%)
22	MA6	AA	1518	22	23,26,27	0.64	0	33,38,41	0.98	1 (3%)
57	PSU	BA	746	57	18,21,22	0.79	0	21,30,33	1.28	4 (19%)
57	PSU	BA	2504	57	18,21,22	0.78	0	21,30,33	1.21	2 (9%)
57	2MG	BA	2445	57	23,26,27	0.55	0	33,38,41	0.84	0
57	PSU	BA	1917	57	18,21,22	0.77	0	21,30,33	1.18	2 (9%)
22	MA6	AA	1519	22	23,26,27	0.66	0	33,38,41	1.07	1 (3%)
22	5MC	AA	967	22	19,22,23	0.67	0	26,32,35	1.49	5 (19%)
22	2MG	AA	1516	22	23,26,27	0.56	0	33,38,41	0.93	1 (3%)
22	4OC	AA	1402	22	20,23,24	0.63	0	25,32,35	1.23	3 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	2MG	BA	1835	57	23,26,27	0.59	0	33,38,41	0.73	0
57	6MZ	BA	2030	57	22,25,26	0.66	0	29,36,39	1.09	2 (6%)
57	OMU	BA	2552	57	19,22,23	0.57	0	25,31,34	0.93	1 (4%)
57	7MG	BA	2069	57	23,26,27	3.90	2 (8%)	27,39,42	1.47	1 (3%)
57	PSU	BA	2457	57	18,21,22	0.78	0	21,30,33	1.20	2 (9%)
24	H2U	A3	21	24	18,21,22	1.05	2 (11%)	19,30,33	0.71	0
57	6MZ	BA	1618	57	22,25,26	0.72	1 (4%)	29,36,39	1.20	3 (10%)
57	OMG	BA	2251	57	23,26,27	0.62	0	32,38,41	1.03	2 (6%)
22	PSU	AA	516	22	18,21,22	0.81	0	21,30,33	1.30	2 (9%)
57	PSU	BA	955	57	18,21,22	0.79	0	21,30,33	1.15	2 (9%)
24	5MU	A3	55	24	19,22,23	0.66	0	27,32,35	1.34	4 (14%)
57	1MG	BA	745	57	23,26,27	0.64	0	33,39,42	1.18	3 (9%)
22	7MG	AA	527	22	23,26,27	3.84	3 (13%)	27,39,42	1.55	2 (7%)
24	PSU	A3	56	24	18,21,22	0.84	0	21,30,33	1.18	2 (9%)
57	PSU	BA	2605	57	18,21,22	0.87	0	21,30,33	1.35	3 (14%)
22	2MG	AA	966	22	23,26,27	0.58	0	33,38,41	0.81	0
57	PSU	BA	1911	57	18,21,22	0.83	0	21,30,33	1.06	2 (9%)
57	2MA	BA	2503	57	22,25,26	0.83	1 (4%)	32,37,40	1.30	4 (12%)
22	5MC	AA	1407	22	19,22,23	0.69	0	26,32,35	1.45	5 (19%)
57	5MC	BA	1962	57	19,22,23	0.72	1 (5%)	26,32,35	1.59	6 (23%)
57	H2U	BA	2449	57	18,21,22	1.16	2 (11%)	19,30,33	1.01	0
24	OMC	A3	33	24	19,22,23	0.69	0	25,31,34	1.13	1 (4%)
57	PSU	BA	2580	57	18,21,22	0.82	0	21,30,33	1.55	4 (19%)
57	5MU	BA	747	57	19,22,23	0.71	0	27,32,35	1.34	3 (11%)
22	UR3	AA	1498	22	19,22,23	0.69	0	26,32,35	1.06	3 (11%)
22	2MG	AA	1207	22	23,26,27	0.60	0	33,38,41	0.72	0
57	5MU	BA	1939	57	19,22,23	0.69	0	27,32,35	1.31	3 (11%)
24	4SU	A3	8	24	18,21,22	1.47	2 (11%)	25,30,33	1.16	2 (8%)

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
57	3TD	BA	1915	57	-	2/7/25/26	0/2/2/2
57	OMC	BA	2498	57	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	MA6	AA	1518	22	-	0/11/29/30	0/3/3/3
57	PSU	BA	746	57	-	0/7/25/26	0/2/2/2
57	PSU	BA	2504	57	-	2/7/25/26	0/2/2/2
57	2MG	BA	2445	57	-	0/9/27/28	0/3/3/3
57	PSU	BA	1917	57	-	0/7/25/26	0/2/2/2
22	MA6	AA	1519	22	-	0/11/29/30	0/3/3/3
22	5MC	AA	967	22	-	0/7/25/26	0/2/2/2
22	2MG	AA	1516	22	-	0/9/27/28	0/3/3/3
22	4OC	AA	1402	22	-	0/9/29/30	0/2/2/2
57	2MG	BA	1835	57	-	0/9/27/28	0/3/3/3
57	6MZ	BA	2030	57	-	0/9/27/28	0/3/3/3
57	OMU	BA	2552	57	-	0/9/27/28	0/2/2/2
57	7MG	BA	2069	57	-	0/7/37/38	0/3/3/3
57	PSU	BA	2457	57	-	0/7/25/26	0/2/2/2
24	H2U	A3	21	24	-	0/7/38/39	0/2/2/2
57	6MZ	BA	1618	57	-	0/9/27/28	0/3/3/3
57	OMG	BA	2251	57	-	0/9/27/28	0/3/3/3
22	PSU	AA	516	22	-	0/7/25/26	0/2/2/2
57	PSU	BA	955	57	-	0/7/25/26	0/2/2/2
24	5MU	A3	55	24	-	0/7/25/26	0/2/2/2
57	1MG	BA	745	57	-	0/7/25/26	0/3/3/3
22	7MG	AA	527	22	-	0/7/37/38	0/3/3/3
24	PSU	A3	56	24	-	2/7/25/26	0/2/2/2
57	PSU	BA	2605	57	-	0/7/25/26	0/2/2/2
22	2MG	AA	966	22	-	0/9/27/28	0/3/3/3
57	PSU	BA	1911	57	-	0/7/25/26	0/2/2/2
57	2MA	BA	2503	57	-	2/7/25/26	0/3/3/3
22	5MC	AA	1407	22	-	0/7/25/26	0/2/2/2
57	5MC	BA	1962	57	-	0/7/25/26	0/2/2/2
57	H2U	BA	2449	57	-	0/7/38/39	0/2/2/2
24	OMC	A3	33	24	-	0/9/27/28	0/2/2/2
57	PSU	BA	2580	57	-	0/7/25/26	0/2/2/2
57	5MU	BA	747	57	-	0/7/25/26	0/2/2/2
22	UR3	AA	1498	22	-	0/7/25/26	0/2/2/2
22	2MG	AA	1207	22	-	0/9/27/28	0/3/3/3
57	5MU	BA	1939	57	-	0/7/25/26	0/2/2/2
24	4SU	A3	8	24	-	0/7/25/26	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	BA	2069	7MG	C8-N9	-18.24	1.34	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	AA	527	7MG	C8-N9	-17.94	1.34	1.45
24	A3	8	4SU	C5-C4	-5.29	1.36	1.42
57	BA	2449	H2U	C4-N3	-3.12	1.32	1.37
57	BA	2449	H2U	C2-N3	-3.00	1.32	1.38
24	A3	21	H2U	C4-N3	-2.77	1.33	1.37
24	A3	21	H2U	C2-N3	-2.63	1.33	1.38
57	BA	2069	7MG	C8-N7	-2.31	1.31	1.42
22	AA	527	7MG	C8-N7	-2.24	1.31	1.42
57	BA	1962	5MC	C5-C4	2.13	1.45	1.44
57	BA	2503	2MA	C4-N3	2.12	1.37	1.34
24	A3	8	4SU	C4-S4	-2.11	1.65	1.68
57	BA	1618	6MZ	C9-N6	2.06	1.48	1.45
22	AA	527	7MG	C5-N7	2.04	1.38	1.35

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	2069	7MG	N9-C8-N7	6.12	112.04	103.37
22	AA	527	7MG	N9-C8-N7	5.87	111.68	103.37
57	BA	1915	3TD	C6-C5-C4	4.02	120.89	118.19
57	BA	745	1MG	N2-C2-N1	4.02	122.02	118.79
57	BA	2580	PSU	C6-C5-C4	3.96	120.85	118.17
57	BA	2605	PSU	C6-C5-C4	3.93	120.82	118.17
57	BA	2498	OMC	O2-C2-N3	-3.80	116.35	122.33
57	BA	1618	6MZ	C9-N6-C6	3.77	126.35	122.85
57	BA	2504	PSU	C6-C5-C4	3.73	120.69	118.17
22	AA	1518	MA6	C2-N1-C6	3.66	120.77	111.83
57	BA	2503	2MA	O4'-C1'-N9	3.52	114.84	108.09
22	AA	516	PSU	C6-C5-C4	3.49	120.53	118.17
57	BA	1917	PSU	C6-C5-C4	3.49	120.53	118.17
57	BA	2030	6MZ	C9-N6-C6	3.41	126.01	122.85
22	AA	1519	MA6	C2-N1-C6	3.40	120.12	111.83
57	BA	747	5MU	C6-C5-C4	3.35	120.78	118.02
57	BA	1962	5MC	N4-C4-N3	-3.34	112.46	118.51
57	BA	955	PSU	C6-C5-C4	3.33	120.42	118.17
24	A3	8	4SU	C5-C4-N3	3.26	117.78	114.75
24	A3	55	5MU	C5M-C5-C6	-3.23	118.48	122.85
22	AA	1407	5MC	O2-C2-N3	-3.21	117.28	122.33
24	A3	33	OMC	O2-C2-N3	-3.20	117.29	122.33
57	BA	1939	5MU	C6-C5-C4	3.15	120.61	118.02
24	A3	56	PSU	C6-C5-C4	3.12	120.28	118.17
57	BA	746	PSU	C6-C5-C4	3.12	120.28	118.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	2503	2MA	N6-C6-N1	-3.07	112.89	117.03
24	A3	55	5MU	C6-C5-C4	3.00	120.49	118.02
57	BA	2457	PSU	C6-C5-C4	2.94	120.16	118.17
57	BA	1962	5MC	C5-C6-N1	-2.93	120.13	123.31
57	BA	1939	5MU	C5M-C5-C6	-2.90	118.92	122.85
57	BA	1962	5MC	CM5-C5-C6	-2.89	118.94	122.85
57	BA	747	5MU	C5M-C5-C6	-2.89	118.94	122.85
22	AA	1516	2MG	N1-C2-N2	-2.88	113.62	116.56
57	BA	1911	PSU	C6-C5-C4	2.87	120.11	118.17
24	A3	8	4SU	C4-N3-C2	-2.86	124.58	127.31
57	BA	745	1MG	C2-N1-C6	2.85	123.37	120.99
22	AA	967	5MC	O2-C2-N3	-2.79	117.94	122.33
22	AA	516	PSU	C5-C6-N1	-2.72	118.36	122.14
57	BA	1962	5MC	O2-C2-N3	-2.72	118.05	122.33
57	BA	2605	PSU	C5-C6-N1	-2.68	118.42	122.14
57	BA	2580	PSU	C3'-C2'-C1'	2.66	104.83	101.69
22	AA	967	5MC	C5-C6-N1	-2.66	120.42	123.31
22	AA	1402	4OC	O2-C2-N3	-2.65	118.14	122.33
57	BA	1618	6MZ	C4-C5-C6	-2.65	114.58	116.78
22	AA	1407	5MC	CM5-C5-C6	-2.64	119.27	122.85
57	BA	1962	5MC	CM5-C5-C4	2.63	124.83	120.51
57	BA	1915	3TD	C5-C6-N1	-2.62	118.51	122.14
57	BA	955	PSU	C5-C6-N1	-2.62	118.51	122.14
57	BA	1618	6MZ	O4'-C1'-N9	2.60	113.08	108.09
57	BA	2504	PSU	C5-C6-N1	-2.59	118.55	122.14
22	AA	967	5MC	N4-C4-N3	-2.56	113.86	118.51
22	AA	1407	5MC	C5-C6-N1	-2.56	120.53	123.31
57	BA	1939	5MU	C5-C6-N1	-2.56	120.53	123.31
57	BA	2580	PSU	C5-C6-N1	-2.53	118.63	122.14
24	A3	56	PSU	C5-C6-N1	-2.52	118.65	122.14
57	BA	2503	2MA	C6-C5-C4	-2.49	113.78	117.18
22	AA	967	5MC	CM5-C5-C6	-2.47	119.51	122.85
22	AA	527	7MG	O4'-C1'-N9	2.42	112.59	109.30
57	BA	1917	PSU	C5-C6-N1	-2.41	118.80	122.14
57	BA	2580	PSU	O4'-C1'-C2'	2.38	108.44	105.15
22	AA	1498	UR3	O4-C4-N3	2.36	122.53	119.66
22	AA	1498	UR3	C4-N3-C2	-2.36	122.68	124.58
57	BA	1962	5MC	C5-C4-N3	2.35	124.16	121.75
57	BA	2605	PSU	O4'-C1'-C2'	2.32	108.36	105.15
57	BA	747	5MU	C5-C6-N1	-2.31	120.81	123.31
57	BA	1911	PSU	C5-C6-N1	-2.30	118.94	122.14
57	BA	745	1MG	N2-C2-N3	-2.30	114.50	119.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AA	1407	5MC	N4-C4-N3	-2.28	114.38	118.51
57	BA	746	PSU	C5-C6-N1	-2.28	118.98	122.14
57	BA	1915	3TD	C4-N3-C2	-2.27	122.21	124.61
22	AA	1407	5MC	CM5-C5-C4	2.22	124.16	120.51
57	BA	2457	PSU	C5-C6-N1	-2.21	119.07	122.14
24	A3	55	5MU	C5-C6-N1	-2.18	120.95	123.31
57	BA	2503	2MA	C2'-C3'-C4'	-2.12	98.52	102.61
57	BA	2030	6MZ	C4-C5-C6	-2.12	115.02	116.78
24	A3	55	5MU	C5M-C5-C4	2.10	121.02	118.78
57	BA	2251	OMG	O3'-C3'-C2'	2.09	117.03	111.19
57	BA	2552	OMU	N3-C2-N1	2.08	117.61	114.89
57	BA	746	PSU	C3'-C2'-C1'	2.08	104.14	101.69
22	AA	967	5MC	CM5-C5-C4	2.07	123.92	120.51
22	AA	1402	4OC	O4'-C1'-N1	2.06	113.03	108.36
22	AA	1498	UR3	O4'-C4'-C3'	2.04	109.21	105.15
57	BA	2251	OMG	C2'-C1'-N9	-2.03	110.38	114.24
57	BA	746	PSU	O4'-C1'-C2'	2.02	107.94	105.15
22	AA	1402	4OC	C2'-C1'-N1	-2.01	110.43	114.24

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A3	56	PSU	O4'-C1'-C5-C4
57	BA	2504	PSU	O4'-C1'-C5-C4
57	BA	2503	2MA	O4'-C1'-N9-C8
57	BA	2503	2MA	O4'-C1'-N9-C4
24	A3	56	PSU	O4'-C1'-C5-C6
57	BA	1915	3TD	O4'-C1'-C5-C6
57	BA	1915	3TD	C2'-C1'-C5-C6
57	BA	2504	PSU	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

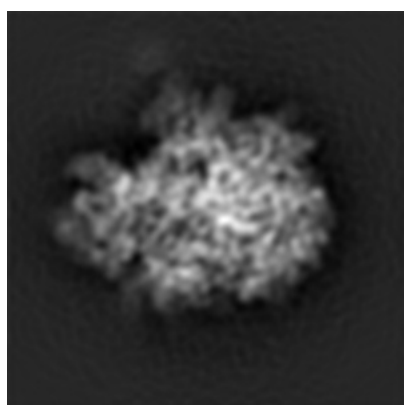
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5562. These allow visual inspection of the internal detail of the map and identification of artifacts.

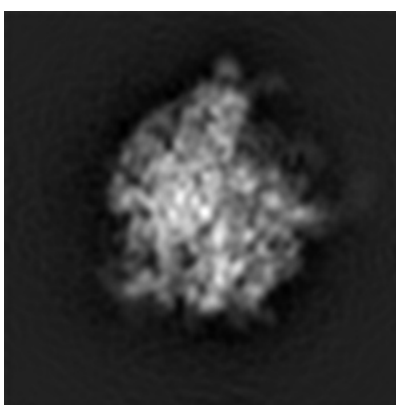
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

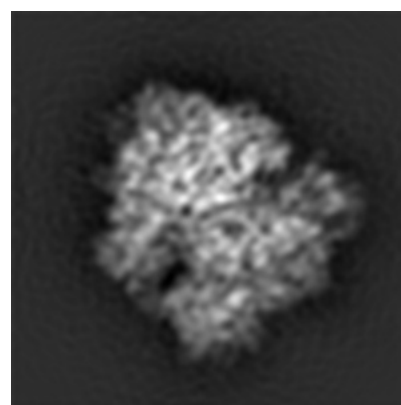
6.1.1 Primary map



X



Y

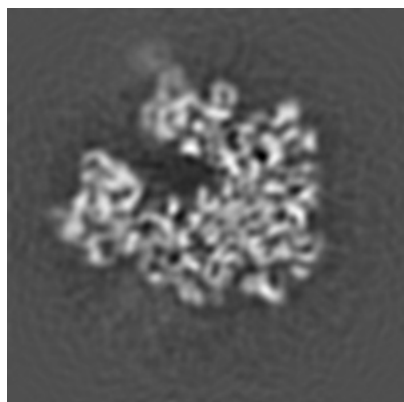


Z

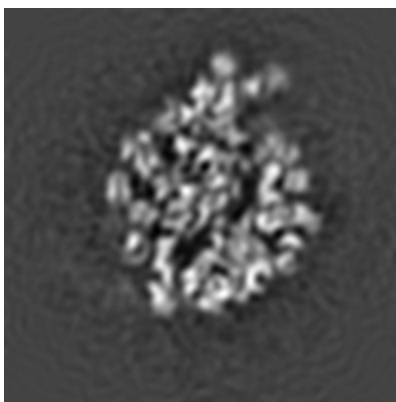
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

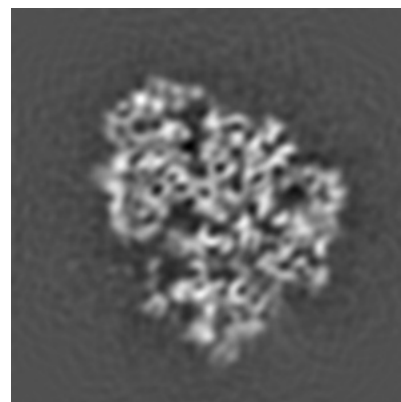
6.2.1 Primary map



X Index: 67



Y Index: 67

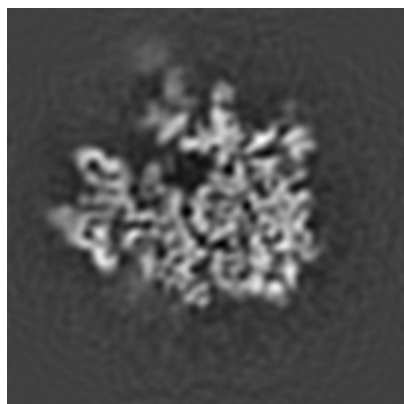


Z Index: 67

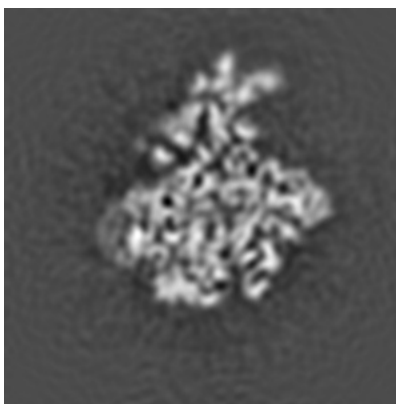
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

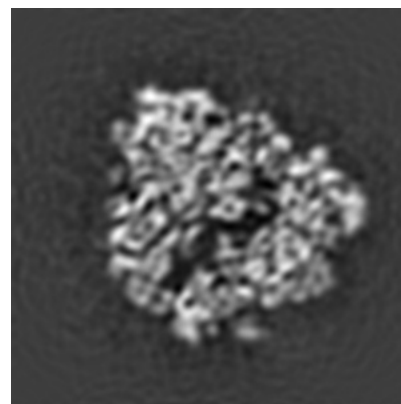
6.3.1 Primary map



X Index: 70



Y Index: 71

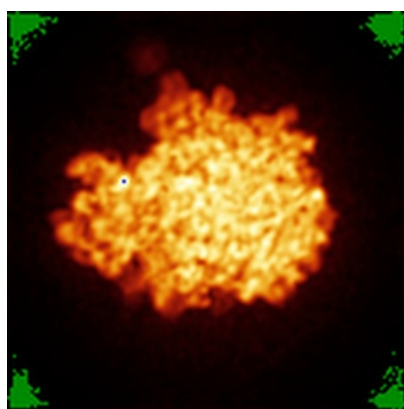


Z Index: 73

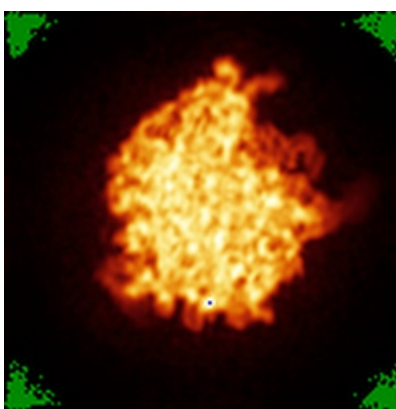
The images above show the largest variance slices of the map in three orthogonal directions.

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

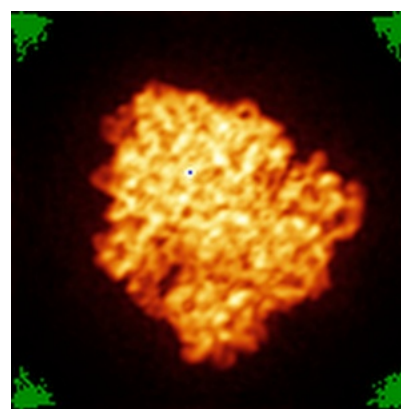
6.4.1 Primary map



X



Y

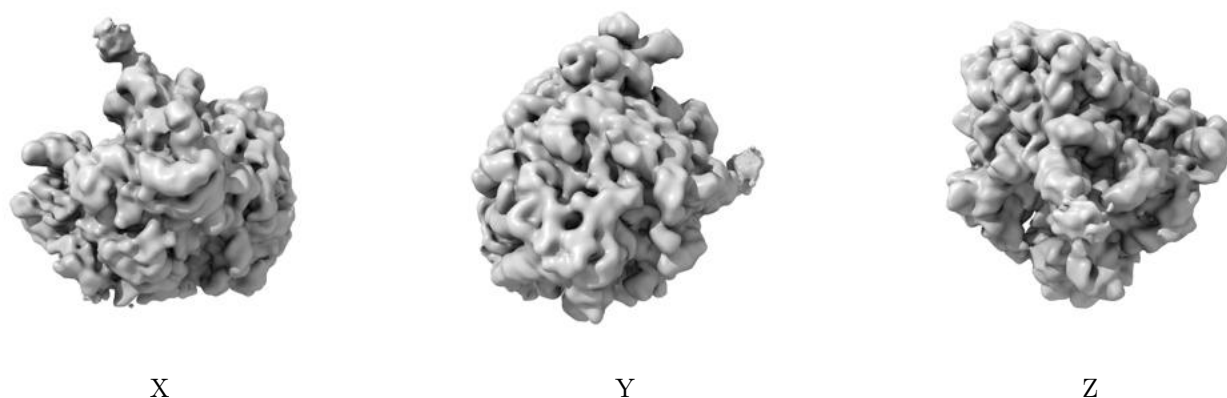


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 22.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

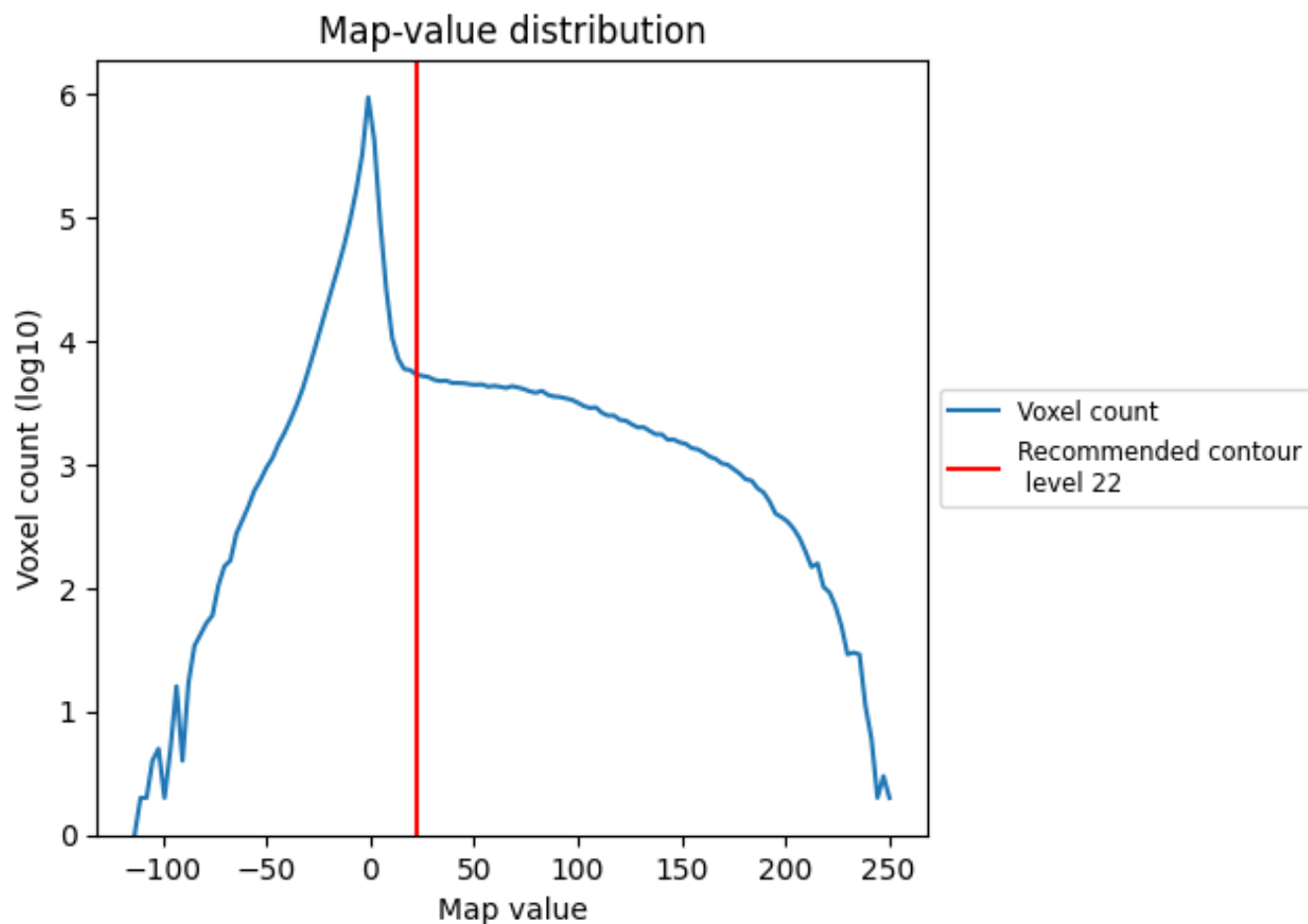
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

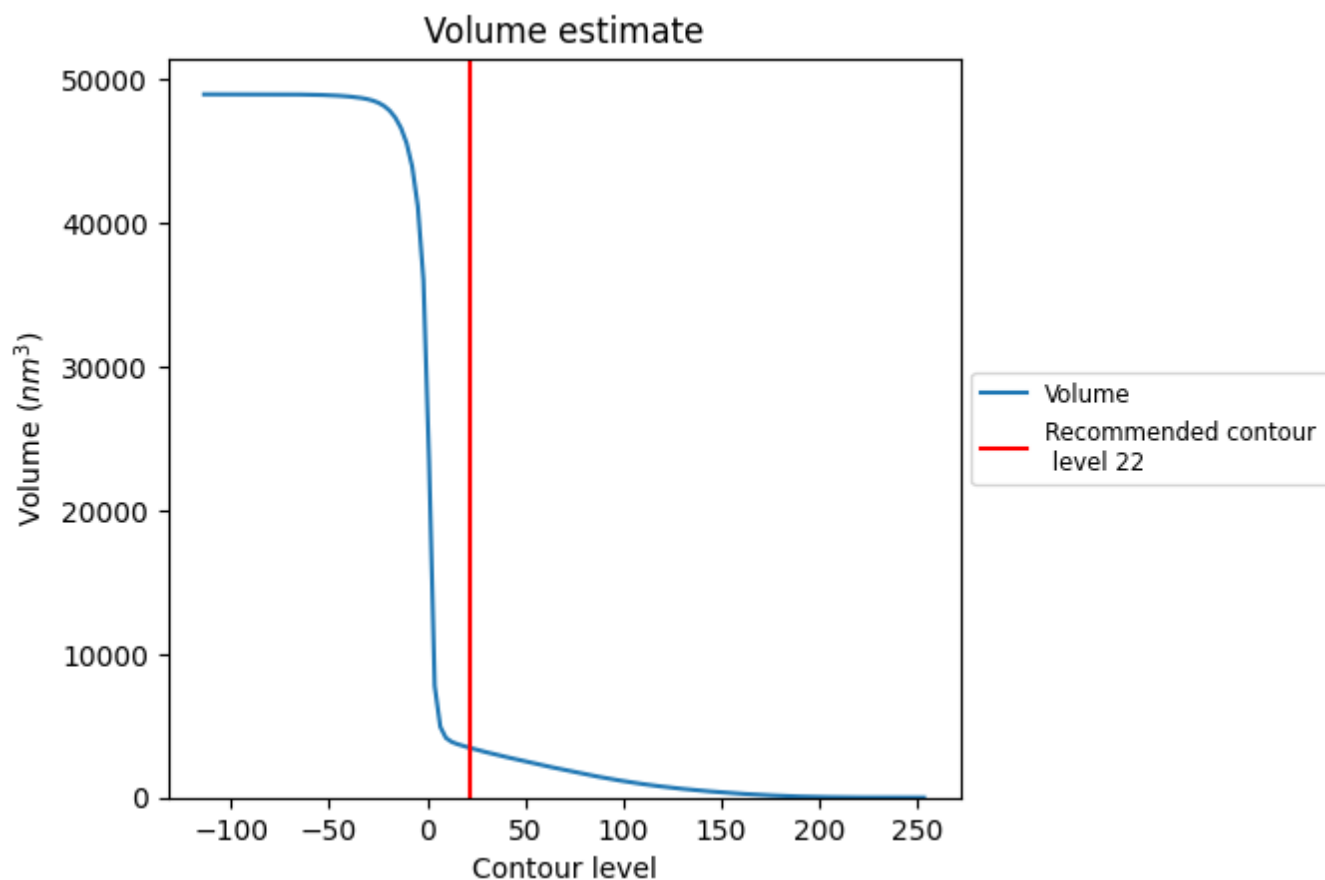
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

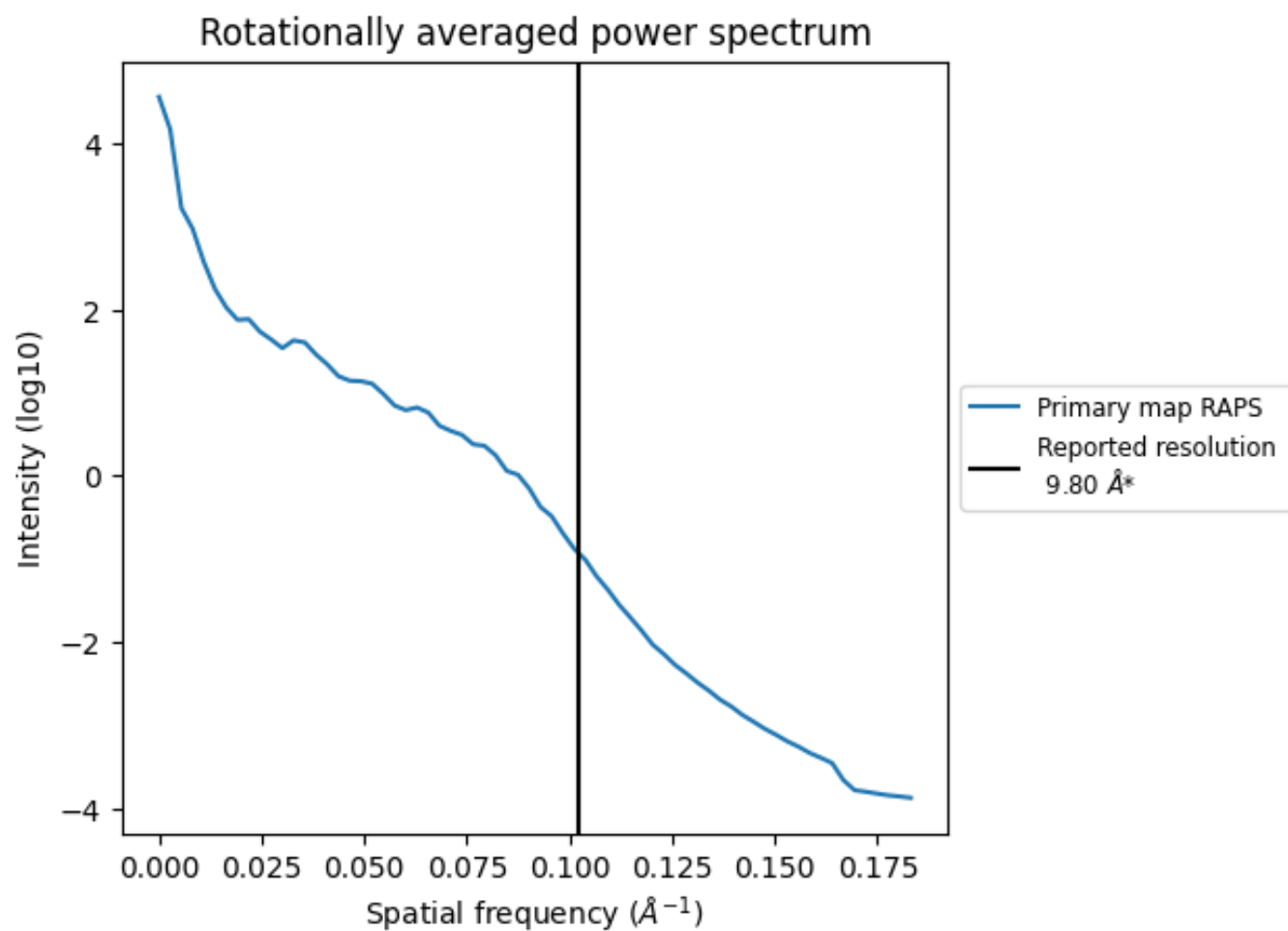
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3450 nm³; this corresponds to an approximate mass of 3116 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.102 Å⁻¹

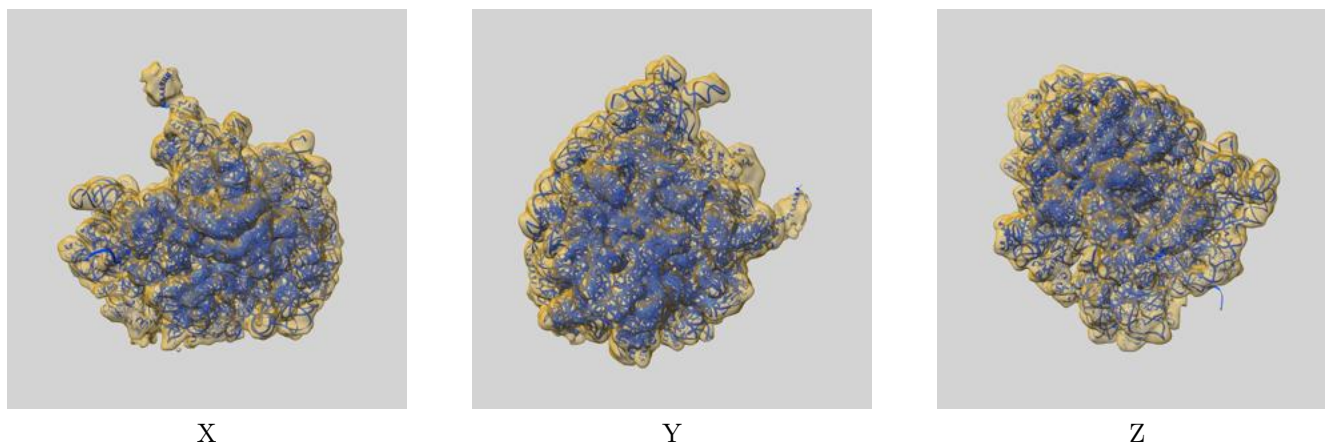
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

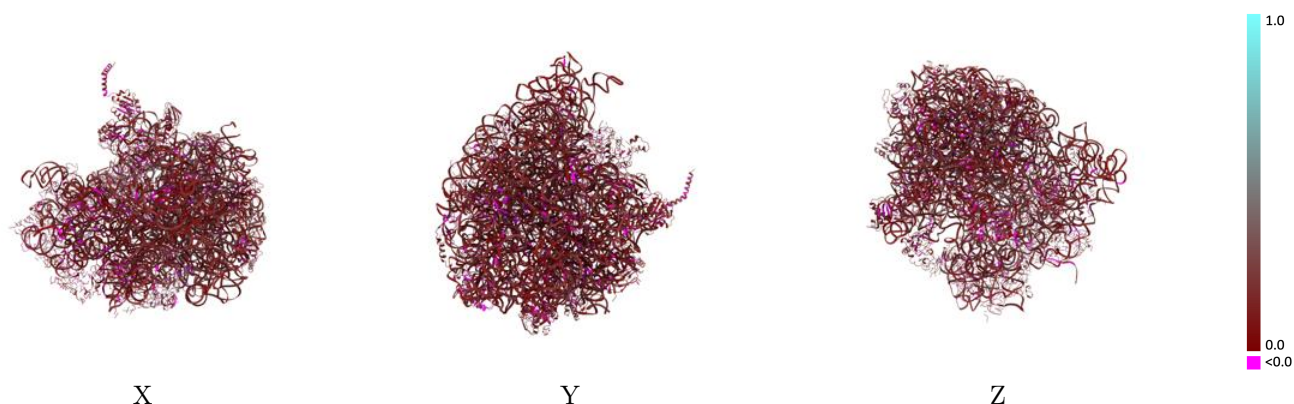
This section contains information regarding the fit between EMDB map EMD-5562 and PDB model 4V6V. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



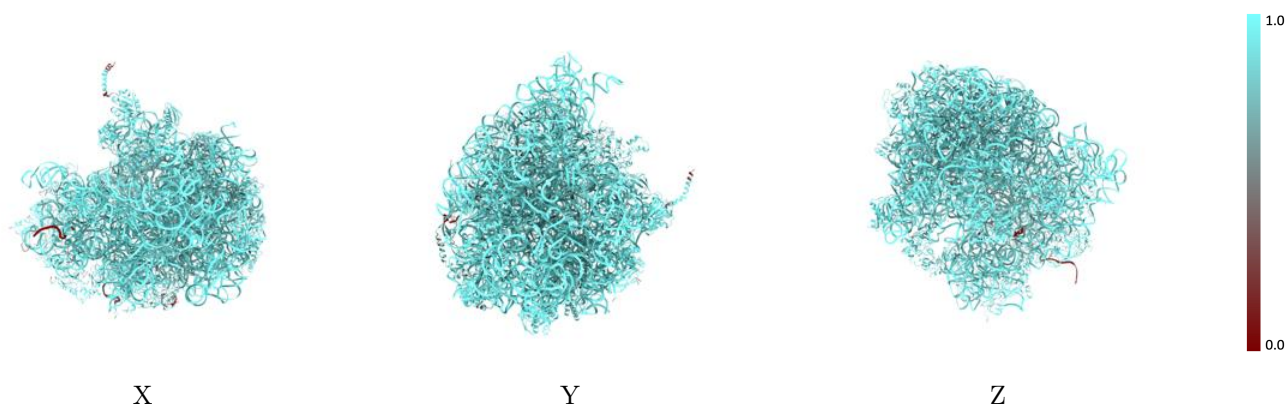
The images above show the 3D surface view of the map at the recommended contour level 22.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



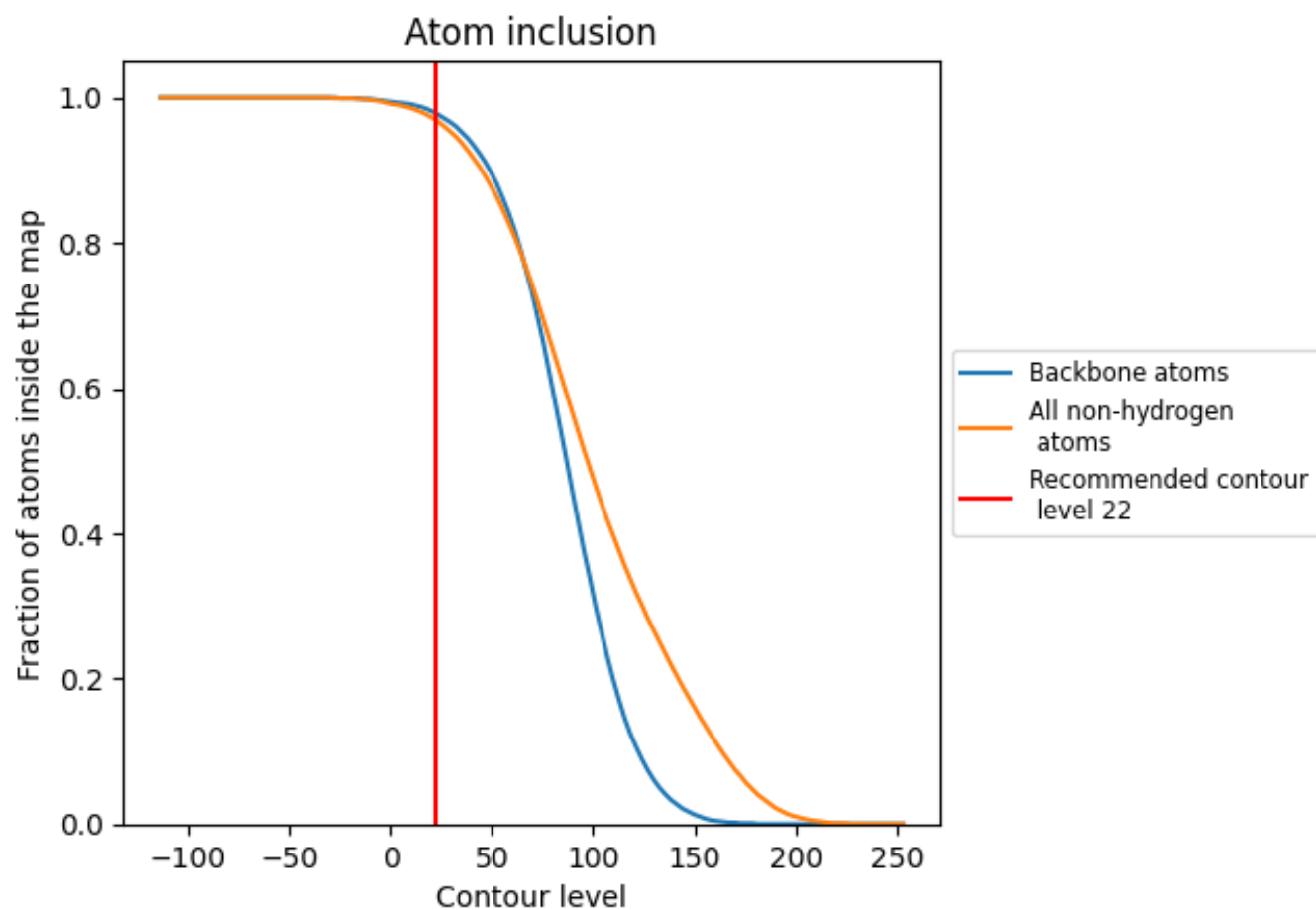
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (22).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 97% 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 (22) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9700	 0.1260
A1	 0.9130	 0.1120
A2	 0.4660	 0.0110
A3	 0.9840	 0.1530
AA	 0.9950	 0.1430
AB	 0.9200	 0.1050
AC	 0.9110	 0.0970
AD	 0.9760	 0.0960
AE	 0.8840	 0.0850
AF	 0.8220	 0.0930
AG	 0.9590	 0.1070
AH	 0.9560	 0.1020
AI	 0.9750	 0.0840
AJ	 0.9580	 0.0780
AK	 0.8950	 0.0910
AL	 0.9260	 0.0940
AM	 0.9720	 0.1100
AN	 0.9470	 0.0640
AO	 0.9800	 0.1040
AP	 0.9730	 0.0620
AQ	 0.9630	 0.1070
AR	 0.9090	 0.0770
AS	 0.9540	 0.0810
AT	 0.9610	 0.1110
AU	 0.8750	 0.0990
B0	 0.9000	 0.0370
B1	 0.9550	 0.0880
B2	 0.9660	 0.1380
B3	 0.9660	 0.1170
B4	 0.8850	 0.0850
B5	 0.9300	 0.0630
B6	 0.9540	 0.0900
B7	 0.9270	 0.0670
B8	 0.9430	 0.0620
B9	 0.9520	 0.0520



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Chain	Atom inclusion	Q-score
BA	 0.9930	 0.1450
BC	 0.8760	 0.0490
BD	 0.9380	 0.0750
BE	 0.9420	 0.0870
BF	 0.9720	 0.0950
BG	 0.9730	 0.0890
BH	 0.9810	 0.1240
BJ	 0.8870	 0.0810
BK	 0.9790	 0.0960
BL	 0.7430	 0.1000
BN	 0.9590	 0.0980
BO	 0.9100	 0.0960
BP	 0.9510	 0.0750
BQ	 0.9500	 0.0920
BR	 0.9520	 0.0900
BS	 0.9760	 0.0940
BT	 0.9350	 0.1020
BU	 0.9660	 0.0980
BV	 0.9400	 0.0990
BW	 0.9250	 0.0900
BX	 0.9600	 0.0890
BY	 0.9600	 0.1060
BZ	 0.9730	 0.1180
Ba	 0.9960	 0.1520