



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 04:22 PM UTC

PDB ID : 7A5H / pdb_00007a5h
EMDB ID : EMD-11643
Title : Structure of the split human mitoribosomal large subunit with rescue factors mtRF-R and MTRES1
Authors : Desai, N.; Yang, H.; Chandrasekaran, V.; Kazi, R.; Minczuk, M.; Ramakrishnan, V.
Deposited on : 2020-08-21
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

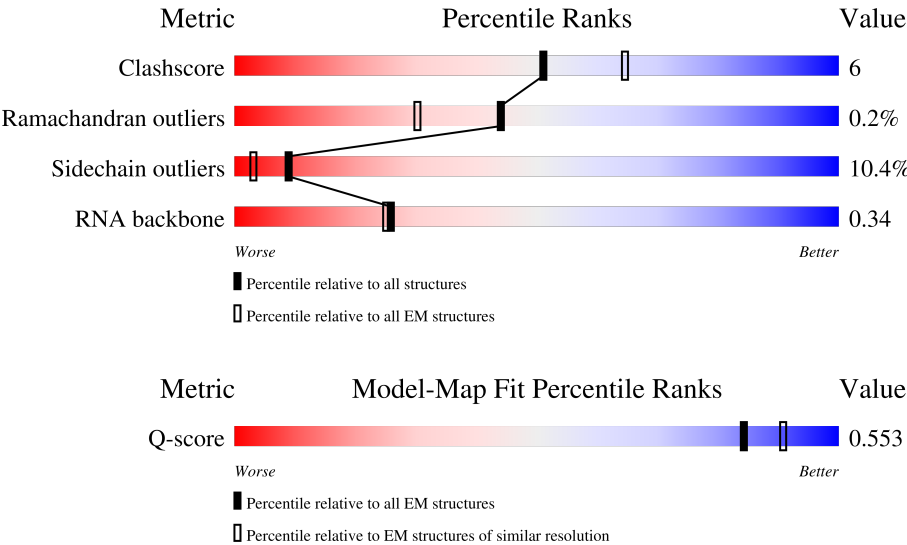
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	D	305	6% 57% 18% 23%
2	E	348	9% 71% 15% 13%
3	F	311	6% 63% 16% 20%

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Mol	Chain	Length	Quality of chain
4	H	267	
5	I	261	
6	J	192	
7	K	178	
8	L	145	
9	M	296	
10	N	251	
11	O	175	
12	P	179	
13	Q	292	
14	R	149	
15	S	205	
16	T	212	
17	U	153	
18	V	216	
19	W	148	
20	X	256	
21	Y	250	
22	Z	161	
23	0	188	
24	1	65	
25	2	92	
26	3	188	
27	5	423	
28	6	380	

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Mol	Chain	Length	Quality of chain
29	7	338	
30	8	206	
31	9	137	
32	a	142	
33	b	155	
34	c	332	
35	d	306	
36	e	279	
37	f	194	
38	g	166	
39	h	158	
40	i	128	
41	j	123	
42	k	112	
43	l	138	
44	m	128	
45	o	102	
46	p	206	
47	q	222	
48	r	196	
49	s	439	
50	t	28	
51	u	234	
52	v	70	
53	w	156	

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Mol	Chain	Length	Quality of chain
54	A	1559	
55	B	73	
56	24	73	
57	Y2	29	
58	C	166	
59	G	240	

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 102610 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 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	236	Total	C	N	O	S	0	0
			1842	1145	373	315	9		

- Molecule 2 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	304	Total	C	N	O	S	0	0
			2396	1539	416	430	11		

- Molecule 3 is a protein called 39S ribosomal protein L4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	250	Total	C	N	O	S	0	0
			2013	1294	365	348	6		

- Molecule 4 is a protein called 39S ribosomal protein L9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	95	Total	C	N	O	S	0	0
			784	498	152	134			

- Molecule 5 is a protein called 39S ribosomal protein L10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	158	Total	C	N	O	S	0	0
			1283	828	235	210	10		

- Molecule 6 is a protein called 39S ribosomal protein L11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	140	Total	C	N	O	S	0	0
			1061	680	192	187	2		

- Molecule 7 is a protein called 39S ribosomal protein L13, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	177	Total	C	N	O	S	0	0
			1451	934	259	251	7		

- Molecule 8 is a protein called 39S ribosomal protein L14, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	115	Total	C	N	O	S	0	0
			889	559	171	154	5		

- Molecule 9 is a protein called 39S ribosomal protein L15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	M	287	Total	C	N	O	S	0	0
			2305	1472	425	402	6		

- Molecule 10 is a protein called 39S ribosomal protein L16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	205	Total	C	N	O	S	0	0
			1654	1056	308	280	10		

- Molecule 11 is a protein called 39S ribosomal protein L17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	O	152	Total	C	N	O	S	0	0
			1245	784	239	215	7		

- Molecule 12 is a protein called Mitochondrial ribosomal protein L18, isoform CRA_b.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	141	Total	C	N	O	S	0	0
			1148	719	221	203	5		

- Molecule 13 is a protein called 39S ribosomal protein L19, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Q	217	Total	C	N	O	S	0	0
			1805	1159	317	320	9		

- Molecule 14 is a protein called 39S ribosomal protein L20, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	R	140	Total	C	N	O	S	0	0
			1153	732	231	186	4		

- Molecule 15 is a protein called 39S ribosomal protein L21, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S	156	Total	C	N	O	S	0	0
			1251	806	222	219	4		

- Molecule 16 is a protein called 39S ribosomal protein L22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	166	Total	C	N	O	S	0	0
			1368	875	254	232	7		

- Molecule 17 is a protein called 39S ribosomal protein L23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	U	152	Total	C	N	O	S	0	0
			1218	772	233	210	3		

- Molecule 18 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	V	202	Total	C	N	O	S	0	0
			1624	1032	291	293	8		

- Molecule 19 is a protein called 39S ribosomal protein L27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	W	109	Total	C	N	O	S	0	0
			859	552	162	142	3		

- Molecule 20 is a protein called 39S ribosomal protein L28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	X	243	Total	C	N	O	S	0	0
			2035	1317	351	362	5		

- Molecule 21 is a protein called 39S ribosomal protein L47, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Y	176	Total	C	N	O	S	0	0
			1517	970	291	252	4		

- Molecule 22 is a protein called 39S ribosomal protein L30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Z	120	Total	C	N	O	S	0	0
			978	626	183	166	3		

- Molecule 23 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	0	108	Total	C	N	O	S	0	0
			880	545	172	157	6		

- Molecule 24 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	1	52	Total	C	N	O	S	0	0
			433	278	83	70	2		

- Molecule 25 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	2	45	Total	C	N	O	S	0	0
			367	227	81	58	1		

- Molecule 26 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	3	95	Total	C	N	O	S	0	0
			831	539	162	127	3		

- Molecule 27 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	5	387	Total	C	N	O	S	0	0
			3156	2039	548	558	11		

- Molecule 28 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	6	324	Total	C	N	O	S	0	0
			2640	1694	470	468	8		

- Molecule 29 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	7	287	Total	C	N	O	S	0	0
			2334	1495	397	425	17		

- Molecule 30 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	8	110	Total	C	N	O	S	0	0
			890	567	155	166	2		

- Molecule 31 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	9	117	Total	C	N	O	S	0	0
			947	614	163	168	2		

- Molecule 32 is a protein called 39S ribosomal protein L42, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	82	Total	C	N	O	S	0	0
			686	434	124	123	5		

- Molecule 33 is a protein called 39S ribosomal protein L43, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	148	Total	C	N	O	S	0	0
			1178	733	229	213	3		

- Molecule 34 is a protein called 39S ribosomal protein L44, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	c	275	Total	C	N	O	S	0	0
			2217	1415	383	410	9		

- Molecule 35 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	d	211	Total	C	N	O	S	0	0
			1741	1123	299	309	10		

- Molecule 36 is a protein called 39S ribosomal protein L46, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	e	217	Total	C	N	O	S	0	0
			1762	1124	310	323	5		

- Molecule 37 is a protein called 39S ribosomal protein L48, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	116	Total	C	N	O	S	0	0
			915	585	152	175	3		

- Molecule 38 is a protein called 39S ribosomal protein L49, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	g	129	Total	C	N	O	S	0	0
			1067	690	185	190	2		

- Molecule 39 is a protein called 39S ribosomal protein L50, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	h	100	Total	C	N	O	S	0	0
			827	524	146	155	2		

- Molecule 40 is a protein called 39S ribosomal protein L51, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	i	97	Total	C	N	O	S	0	0
			827	532	165	126	4		

- Molecule 41 is a protein called cDNA FLJ76418, highly similar to Homo sapiens mitochondrial ribosomal protein L52 (MRPL52), transcript variant 1, mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	j	85	Total	C	N	O	S	0	0
			684	423	133	126	2		

- Molecule 42 is a protein called 39S ribosomal protein L53, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	k	80	Total	C	N	O	S	0	0
			627	392	116	114	5		

- Molecule 43 is a protein called 39S ribosomal protein L54, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	l	23	Total	C	N	O	0	0
			221	137	52	32		

- Molecule 44 is a protein called 39S ribosomal protein L55, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	m	45	Total	C	N	O	S	0	0
			372	232	76	62	2		

- Molecule 45 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	91	Total	C	N	O	S	0	0
			771	487	156	125	3		

- Molecule 46 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	p	127	Total	C	N	O	S	0	0
			1058	661	201	192	4		

- Molecule 47 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	q	128	Total	C	N	O	S	0	0
			1076	671	208	192	5		

- Molecule 48 is a protein called 39S ribosomal protein S18a, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	r	146	Total	C	N	O	S	0	0
			1203	764	232	199	8		

- Molecule 49 is a protein called 39S ribosomal protein S30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	s	370	Total	C	N	O	S	0	0
			3036	1946	542	534	14		

- Molecule 50 is a protein called Unknown protein/protein extension.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	t	28	Total	C	N	O	0	0
			140	84	28	28		

- Molecule 51 is a protein called Mitochondrial assembly of ribosomal large subunit protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	u	111	Total	C	N	O	S	0	0
			927	595	155	167	10		

- Molecule 52 is a protein called MIEF1 upstream open reading frame protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	v	69	Total	C	N	O	0	0
			588	372	116	100		

- Molecule 53 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	w	79	Total	C	N	O	S	0	0
			638	410	95	128	5		

- Molecule 54 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	A	1457	Total	C	N	O	P	0	0
			30945	13883	5590	10015	1457		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3107	U	UNK	conflict	GB 1025814679

- Molecule 55 is a RNA chain called mt-tRNAVal.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	B	56	Total	C	N	O	P	0	0
			1191	534	214	387	56		

- Molecule 56 is a RNA chain called mt-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	24	73	Total	C	N	O	P	0	0
			1547	696	280	499	72		

- Molecule 57 is a protein called nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	Y2	29	Total	C	N	O	0	0
			157	96	32	29		

- Molecule 58 is a protein called Probable peptide chain release factor C12orf65, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	C	114	Total	C	N	O	S	1	0
			928	578	177	171	2		

- Molecule 59 is a protein called Mitochondrial transcription rescue factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	G	96	Total	C	N	O	S	0	0
			809	523	142	143	1		

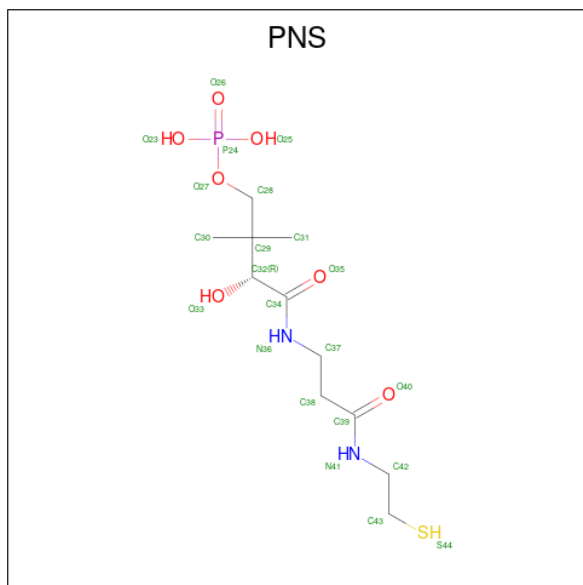
- Molecule 60 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
60	D	1	Total	Mg	0
			1	1	
60	W	1	Total	Mg	0
			1	1	
60	g	1	Total	Mg	0
			1	1	
60	A	89	Total	Mg	0
			89	89	

- Molecule 61 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
61	0	1	Total	Zn	0
			1	1	
61	r	1	Total	Zn	0
			1	1	

- Molecule 62 is 4'-PHOSPHOPANTETHEINE (CCD ID: PNS) (formula: $C_{11}H_{23}N_2O_7PS$).

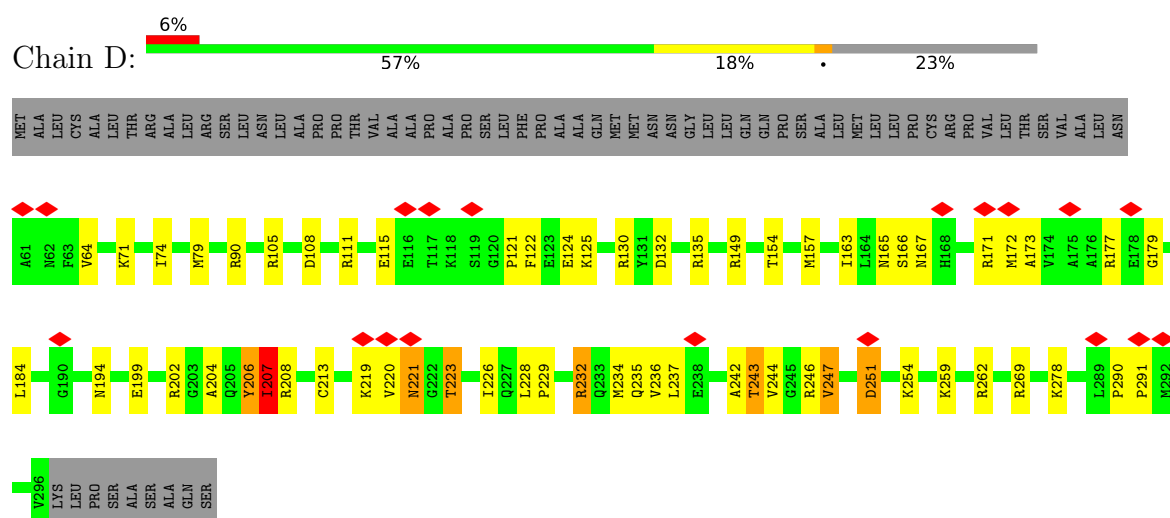


Mol	Chain	Residues	Atoms						AltConf
62	v	1	Total	C	N	O	P	S	0
			21	11	2	6	1	1	

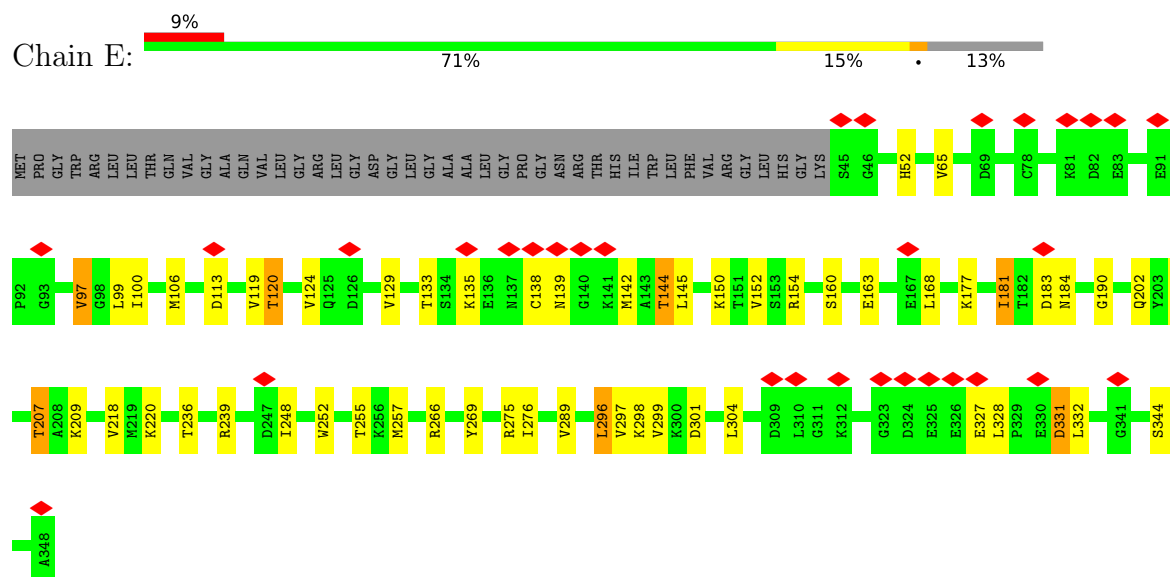
3 Residue-property plots

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

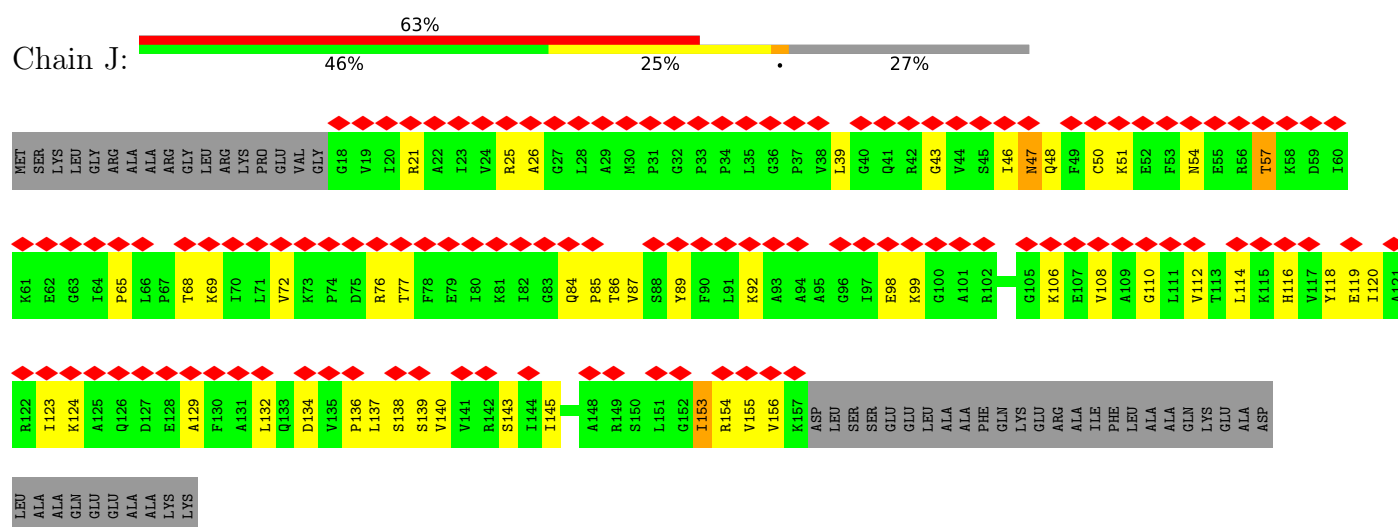
- Molecule 1: 39S ribosomal protein L2, mitochondrial



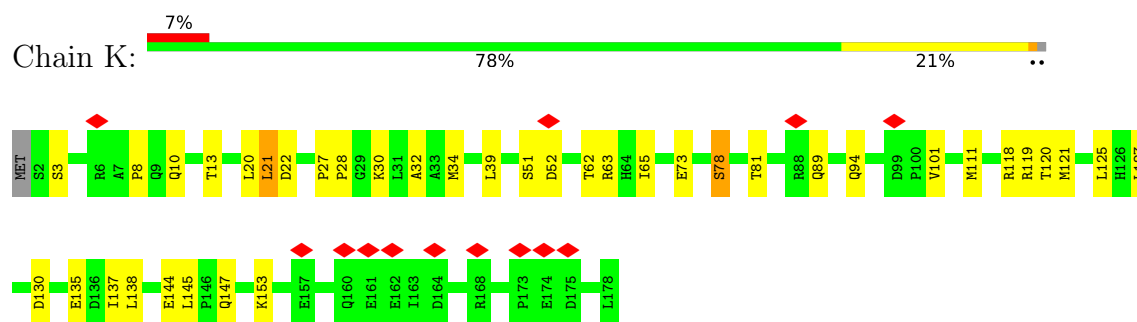
- Molecule 2: 39S ribosomal protein L3, mitochondrial



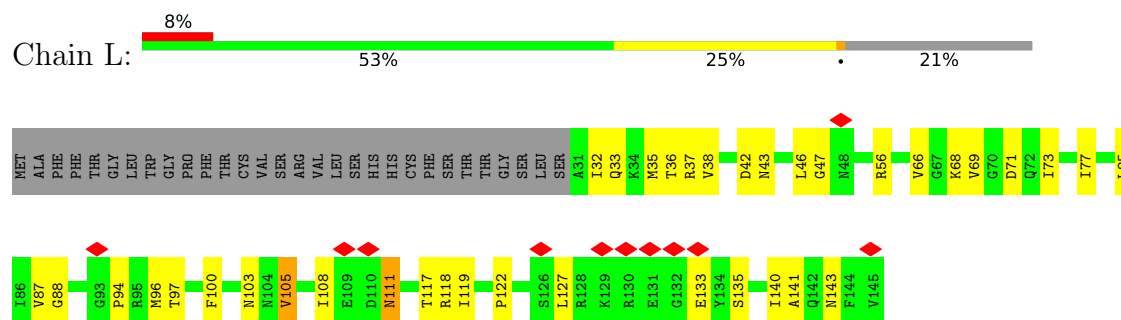
- Molecule 3: 39S ribosomal protein L4, mitochondrial



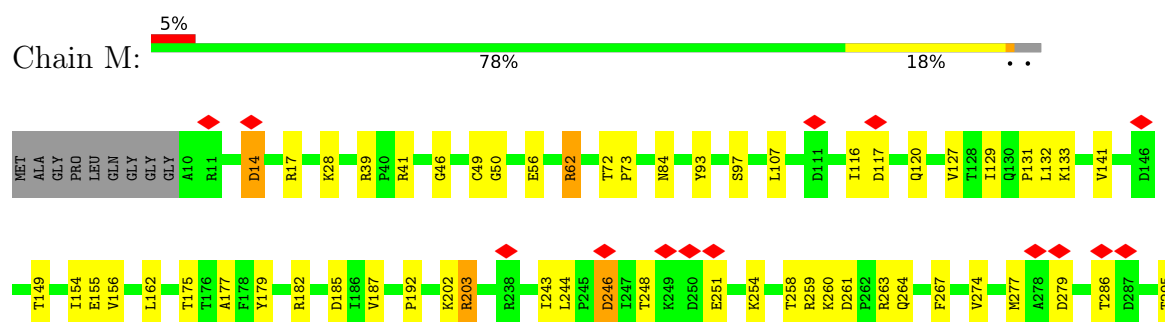
- Molecule 7: 39S ribosomal protein L13, mitochondrial



- Molecule 8: 39S ribosomal protein L14, mitochondrial

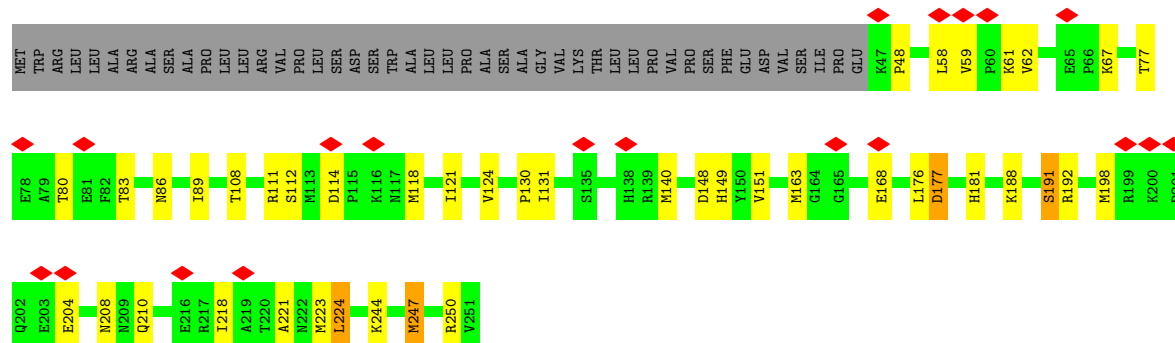


- Molecule 9: 39S ribosomal protein L15, mitochondrial

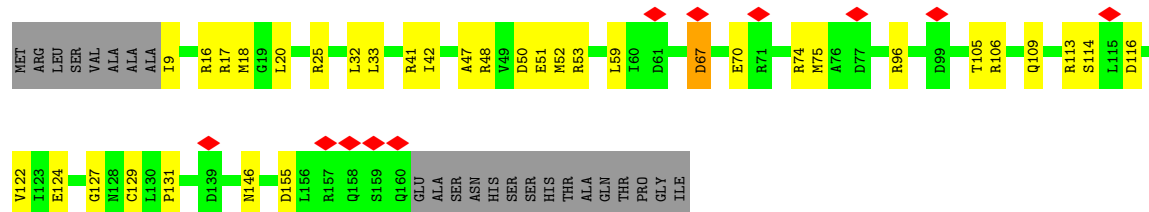




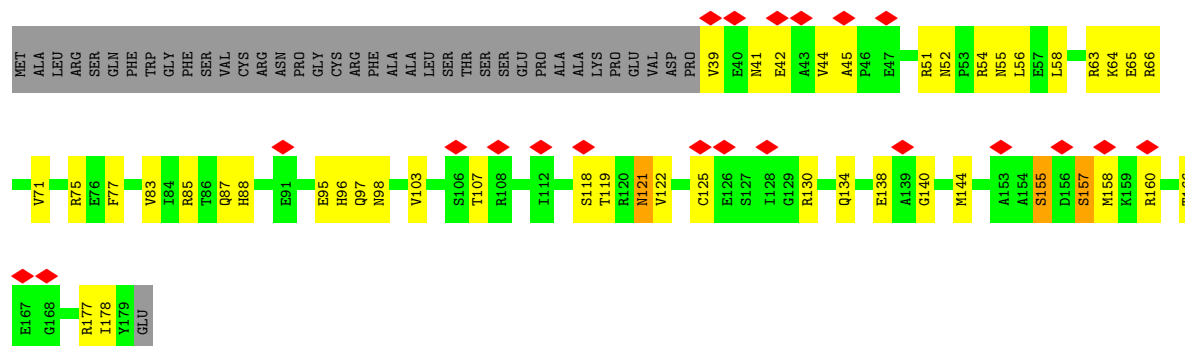
- Molecule 10: 39S ribosomal protein L16, mitochondrial



- Molecule 11: 39S ribosomal protein L17, mitochondrial

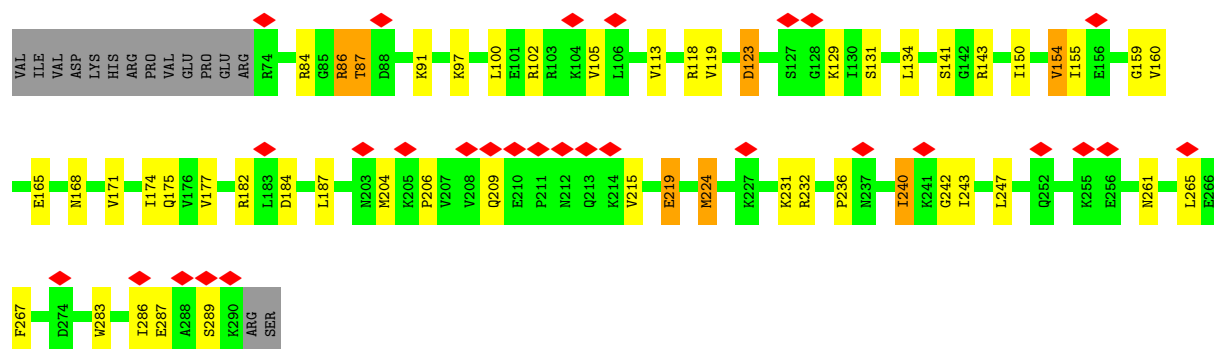


- Molecule 12: Mitochondrial ribosomal protein L18, isoform CRA_b

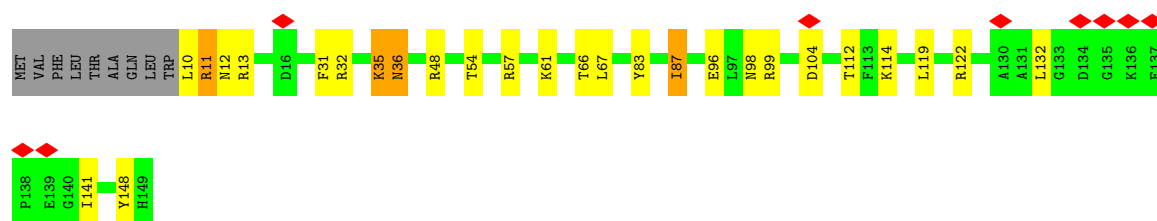
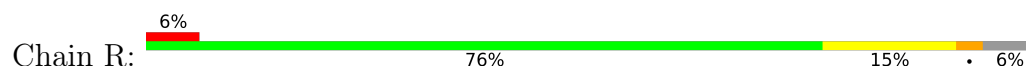


- Molecule 13: 39S ribosomal protein L19, mitochondrial

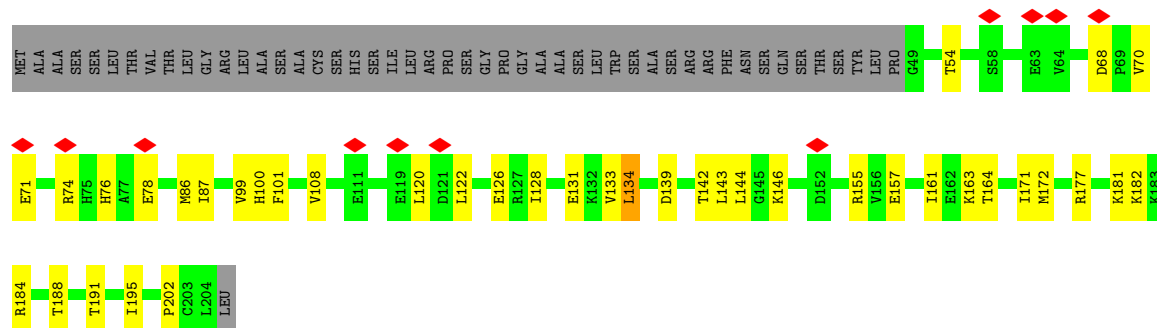




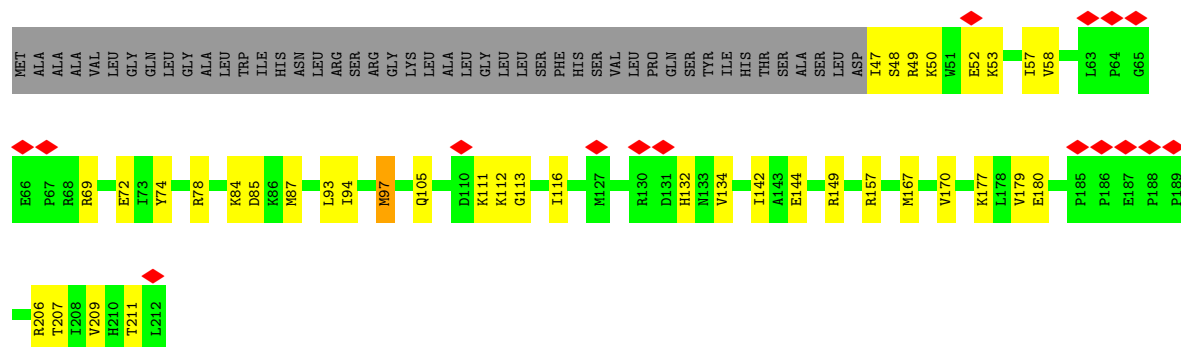
- Molecule 14: 39S ribosomal protein L20, mitochondrial



- Molecule 15: 39S ribosomal protein L21, mitochondrial

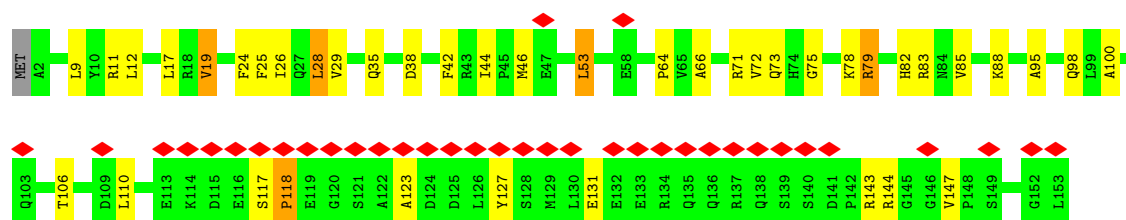


- Molecule 16: 39S ribosomal protein L22, mitochondrial



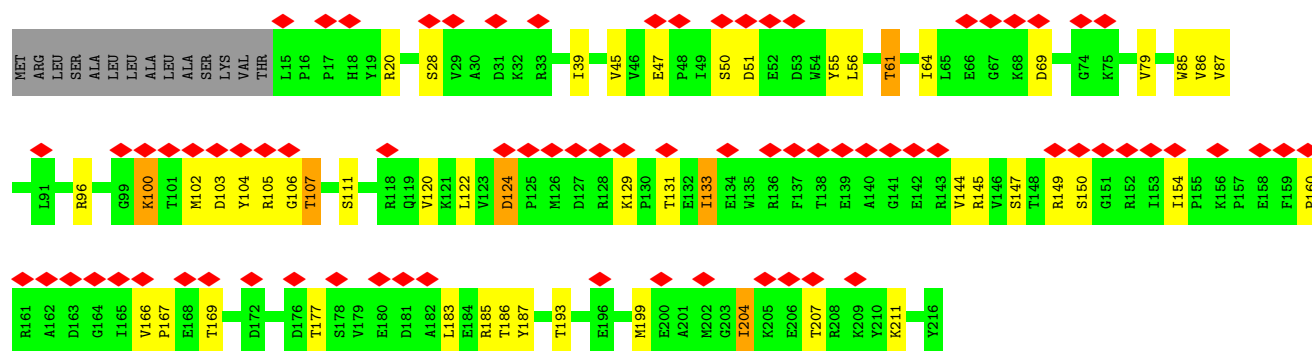
- Molecule 17: 39S ribosomal protein L23, mitochondrial

Chain U: 



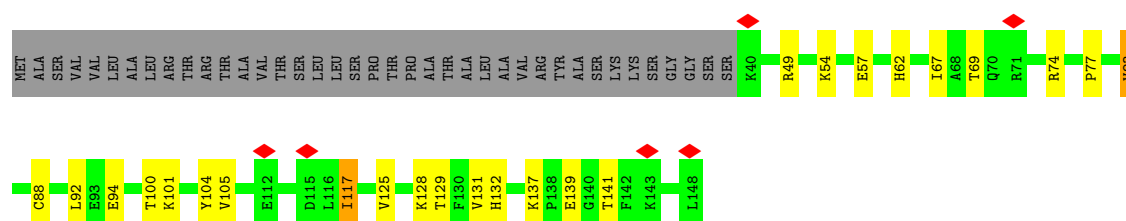
- Molecule 18: 39S ribosomal protein L24, mitochondrial

Chain V: 



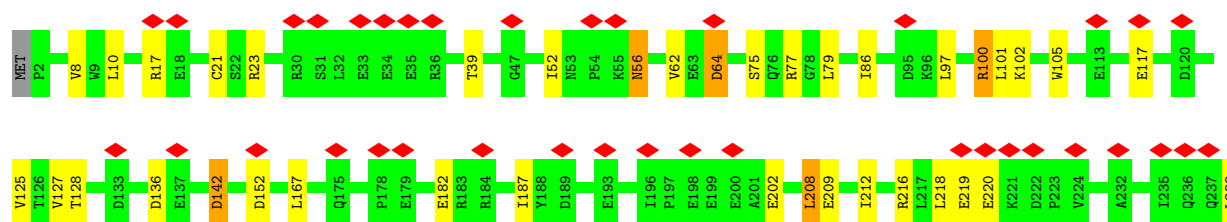
- Molecule 19: 39S ribosomal protein L27, mitochondrial

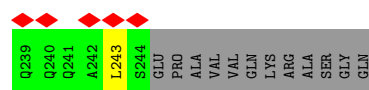
Chain W: 



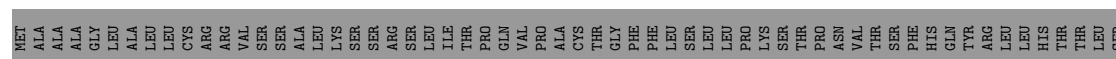
- Molecule 20: 39S ribosomal protein L28, mitochondrial

Chain X: 

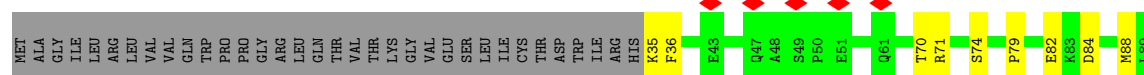




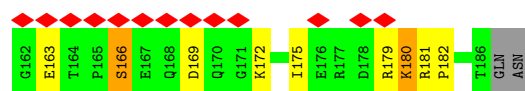
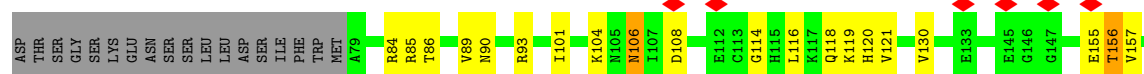
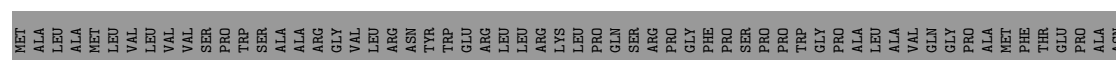
- Molecule 21: 39S ribosomal protein L47, mitochondrial



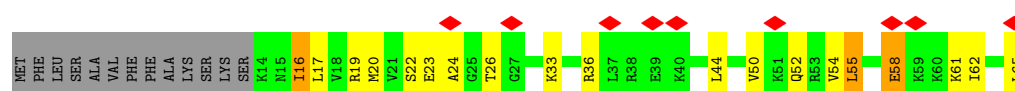
- Molecule 22: 39S ribosomal protein L30, mitochondrial

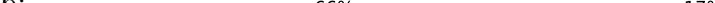


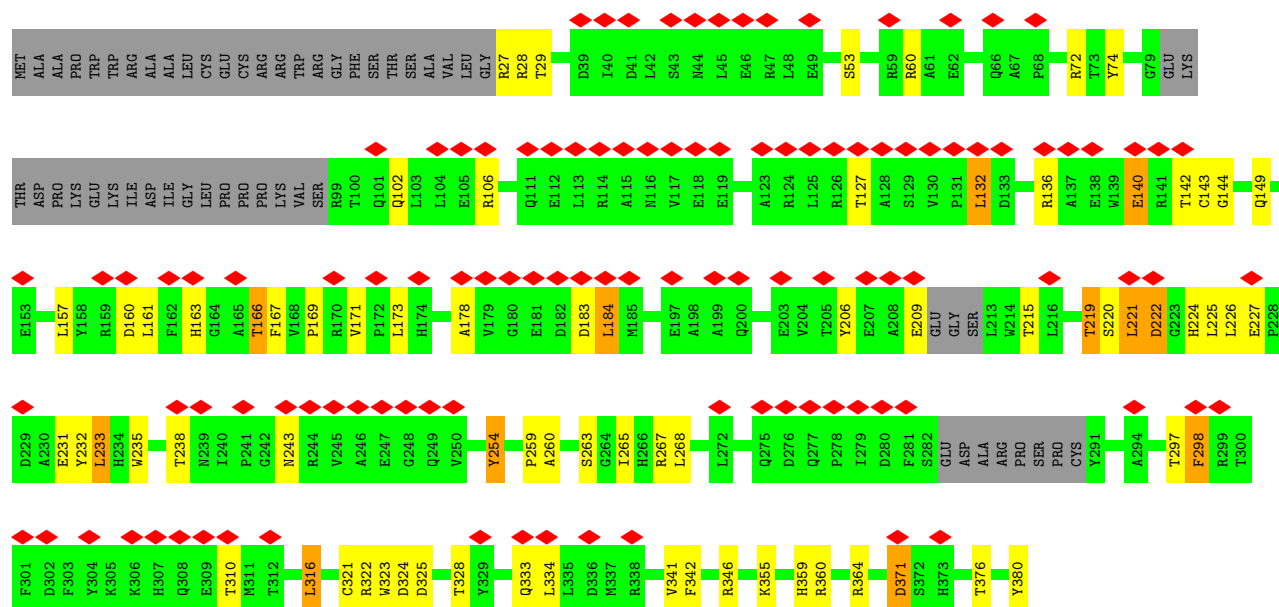
- Molecule 23: 39S ribosomal protein L32, mitochondrial



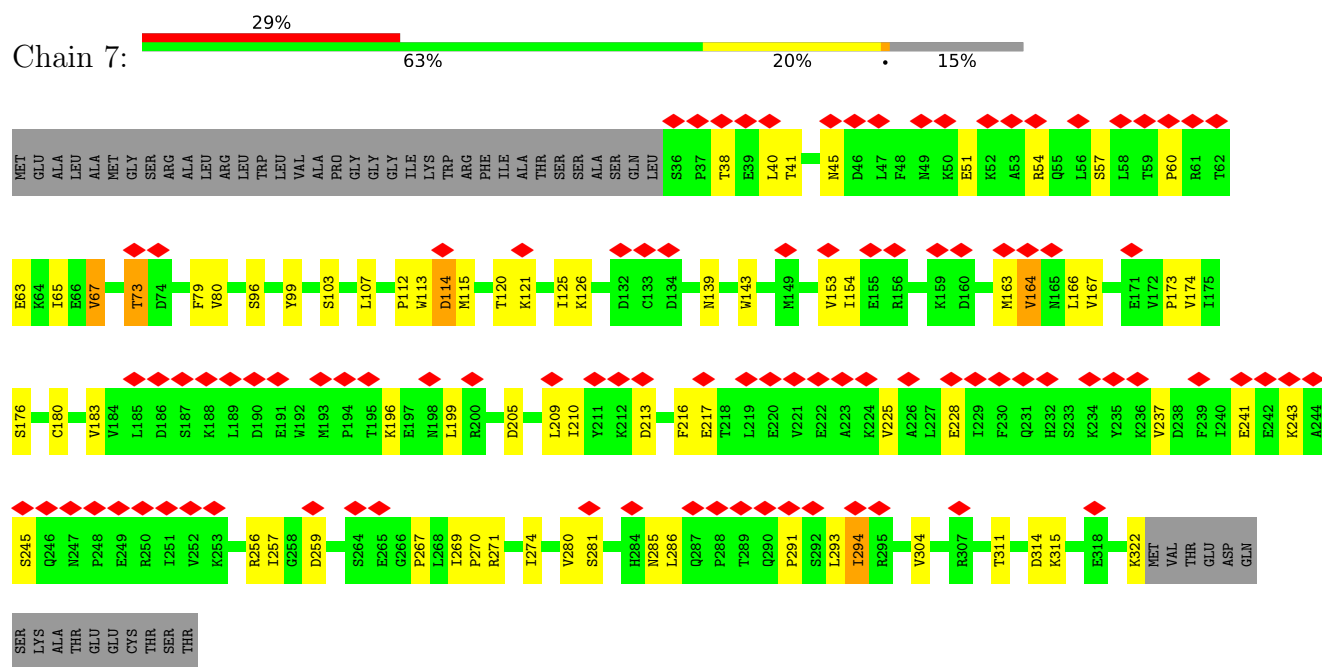
- Molecule 24: 39S ribosomal protein L33, mitochondrial



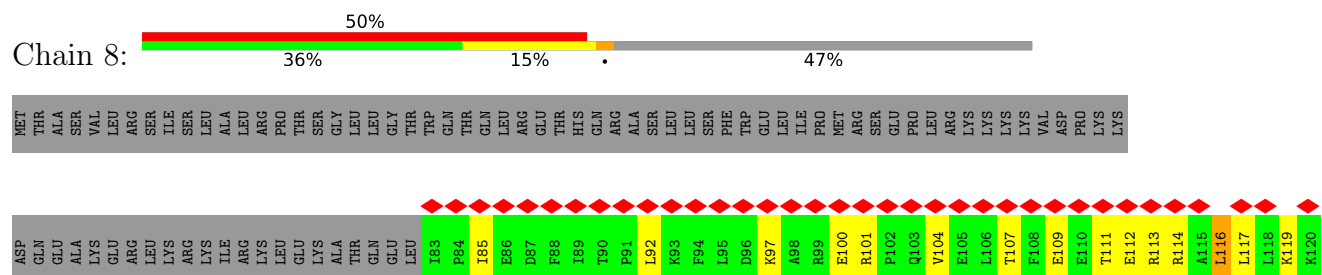
- Chain 6: 



• Molecule 29: 39S ribosomal protein L39, mitochondrial

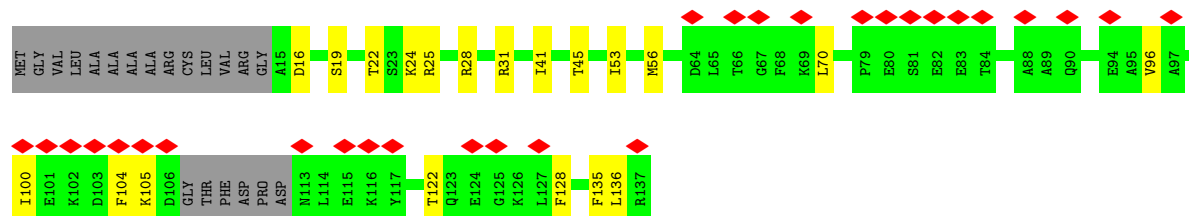


• Molecule 30: 39S ribosomal protein L40, mitochondrial

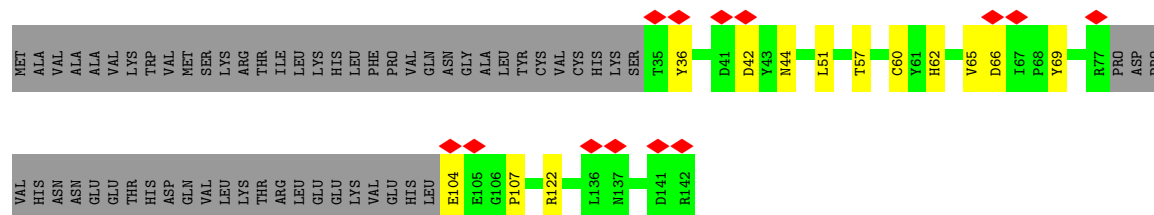




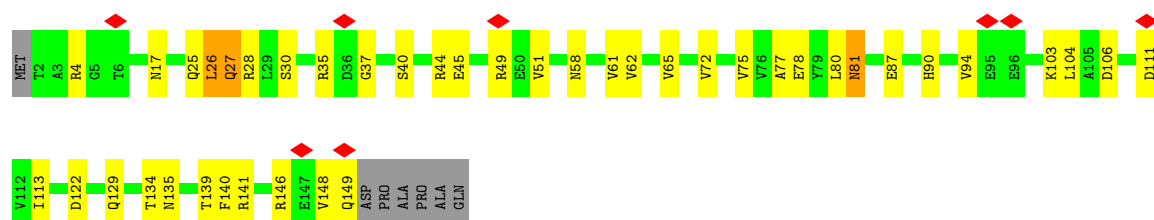
• Molecule 31: 39S ribosomal protein L41, mitochondrial



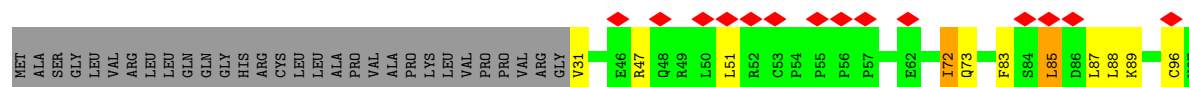
• Molecule 32: 39S ribosomal protein L42, mitochondrial

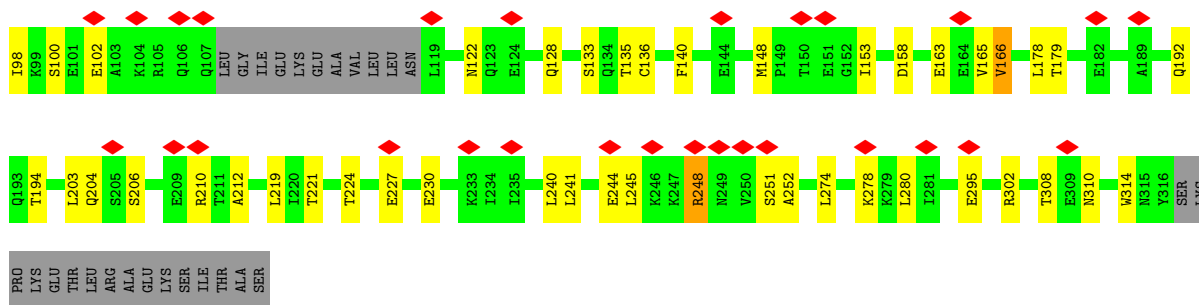


• Molecule 33: 39S ribosomal protein L43, mitochondrial

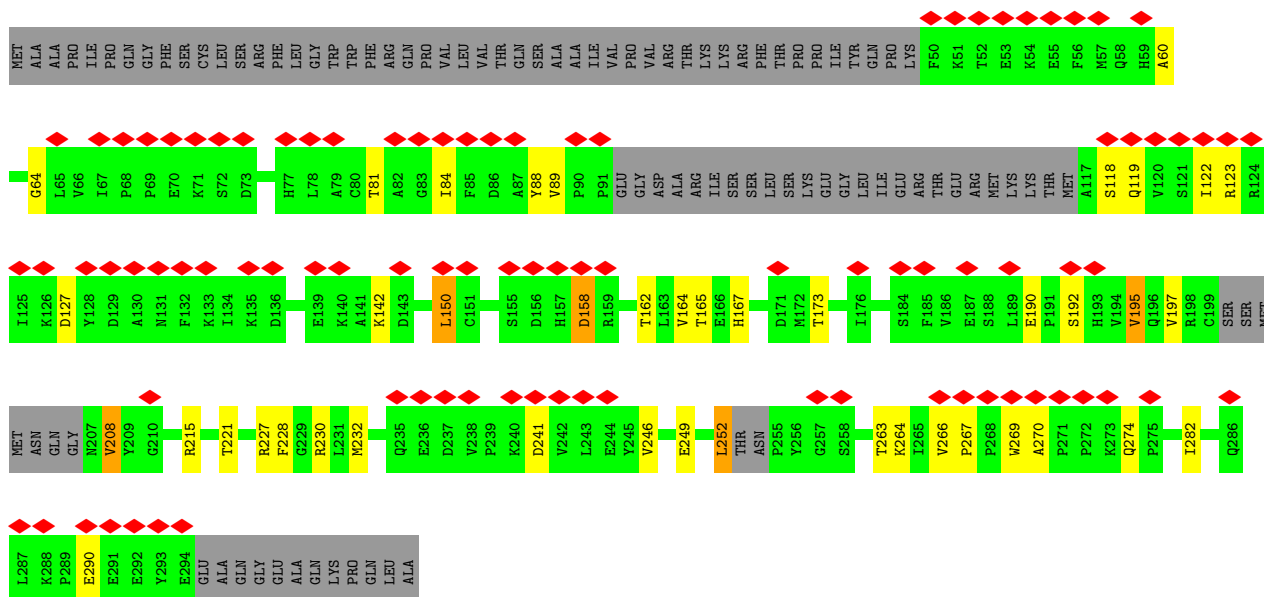


• Molecule 34: 39S ribosomal protein L44, mitochondrial

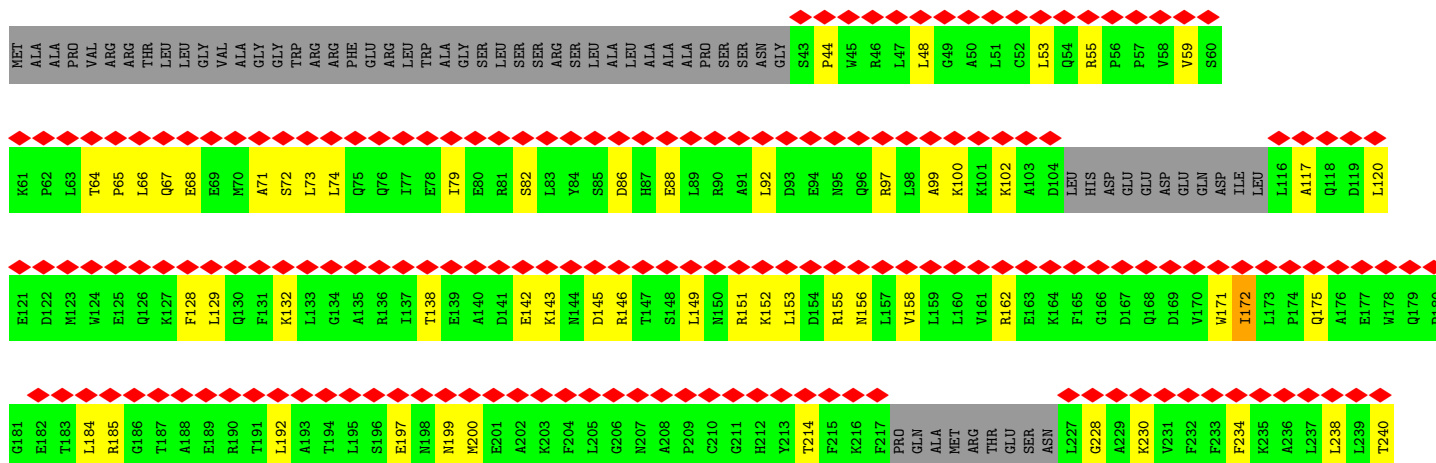
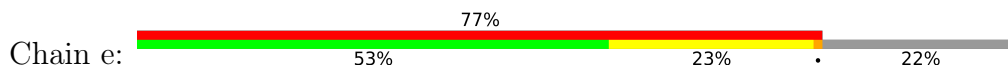




- Molecule 35: 39S ribosomal protein L45, mitochondrial

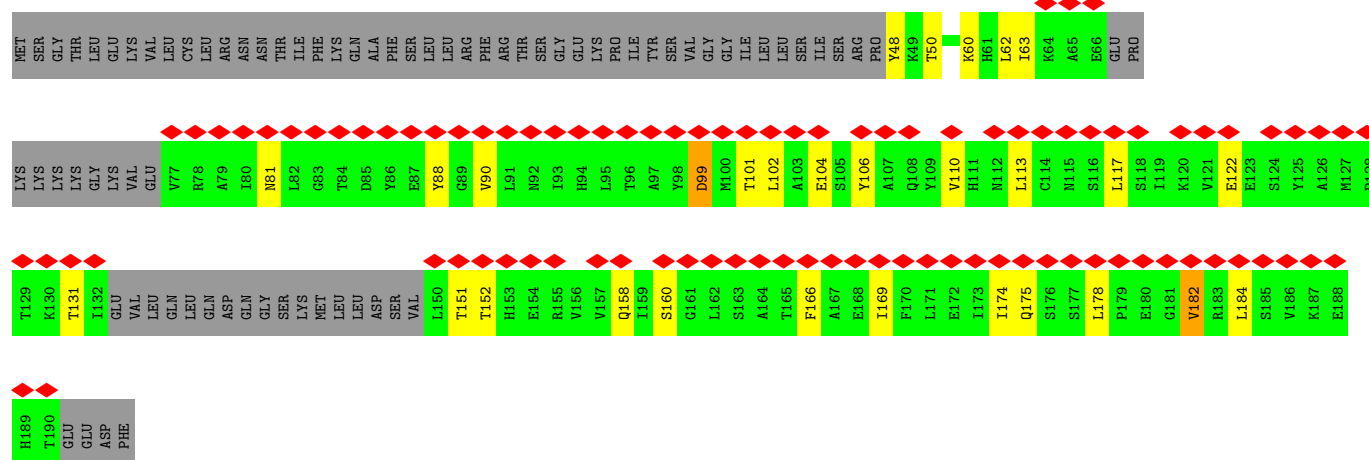


- Molecule 36: 39S ribosomal protein L46, mitochondrial

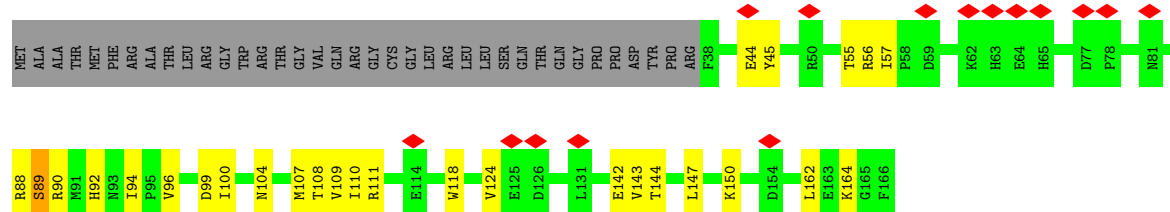




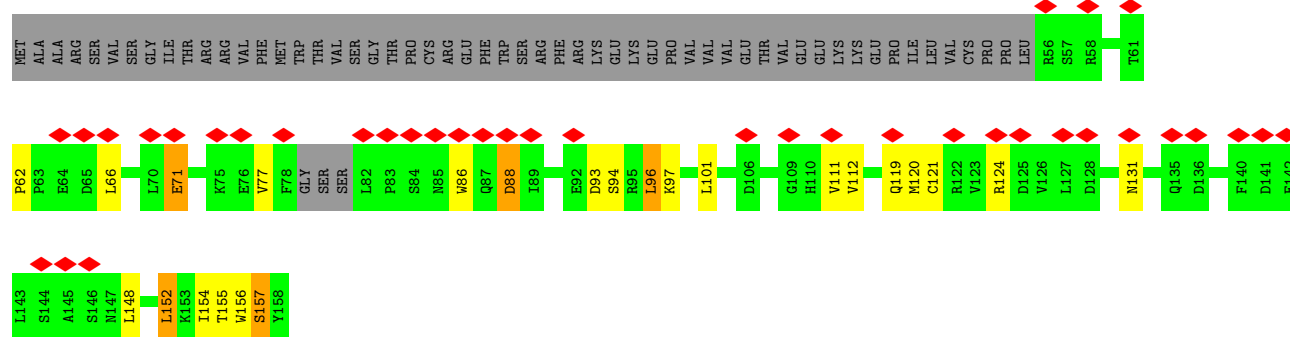
- Molecule 37: 39S ribosomal protein L48, mitochondrial



- Molecule 38: 39S ribosomal protein L49, mitochondrial



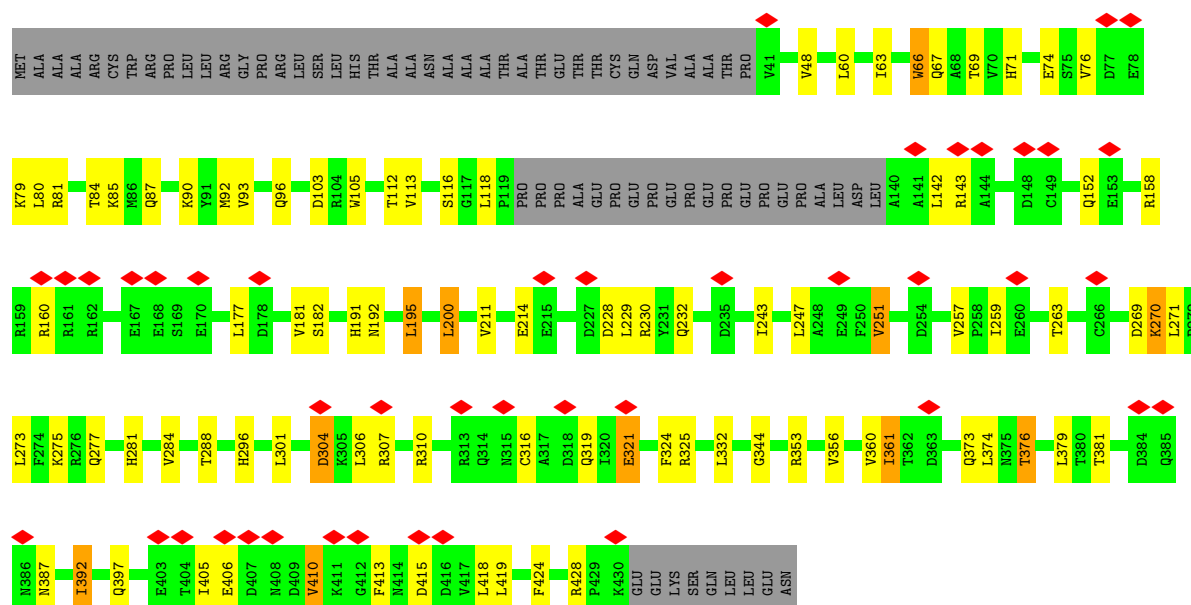
- Molecule 39: 39S ribosomal protein L50, mitochondrial



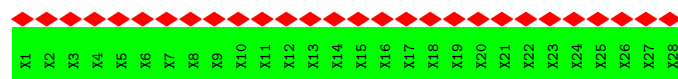
- Molecule 40: 39S ribosomal protein L51, mitochondrial



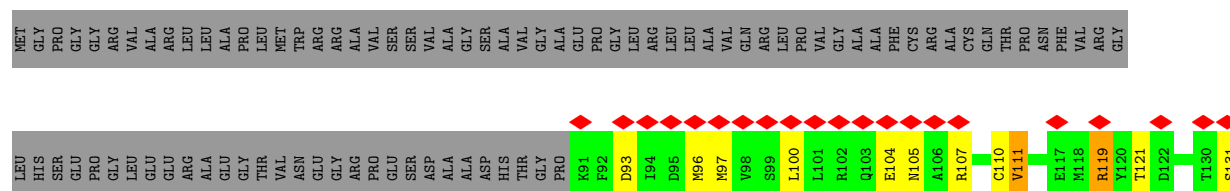
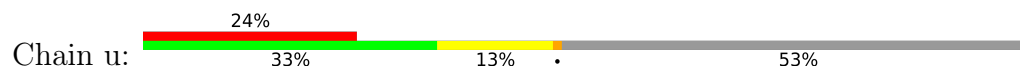
- Molecule 49: 39S ribosomal protein S30, mitochondrial



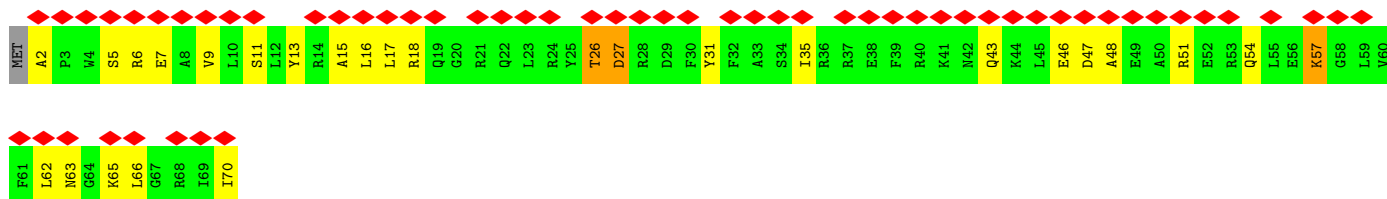
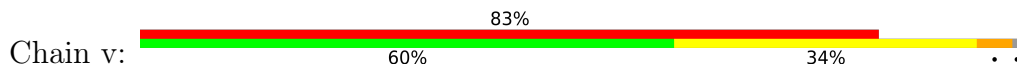
- Molecule 50: Unknown protein/protein extension



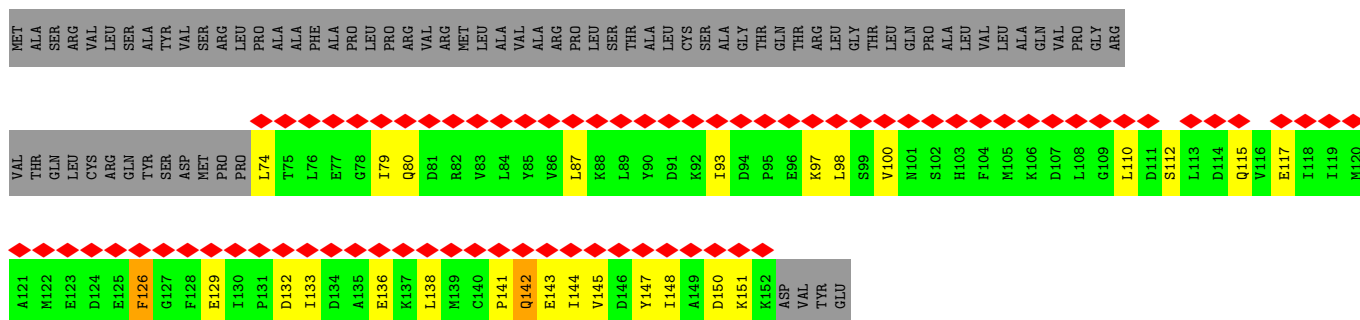
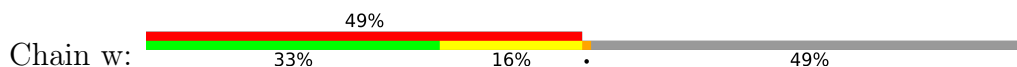
- Molecule 51: Mitochondrial assembly of ribosomal large subunit protein 1



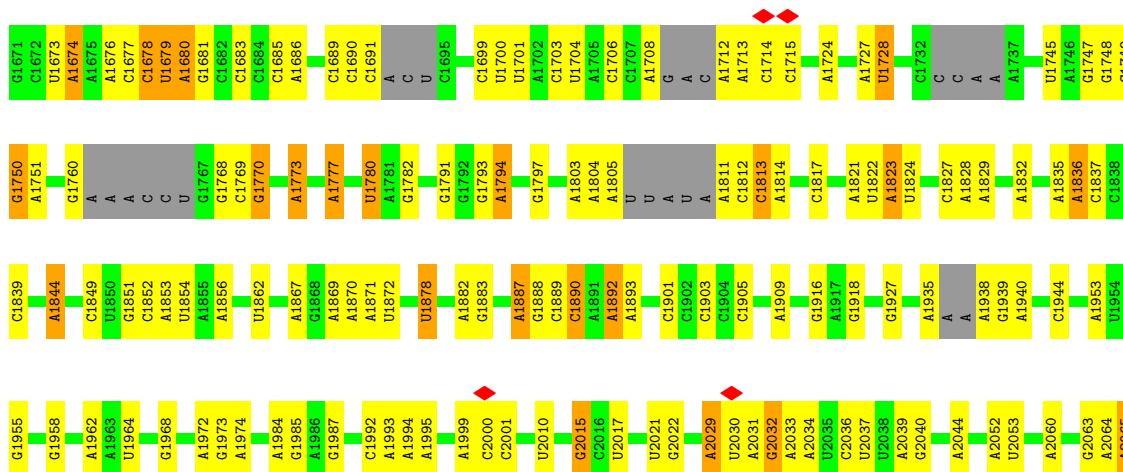
- Molecule 52: MIEF1 upstream open reading frame protein

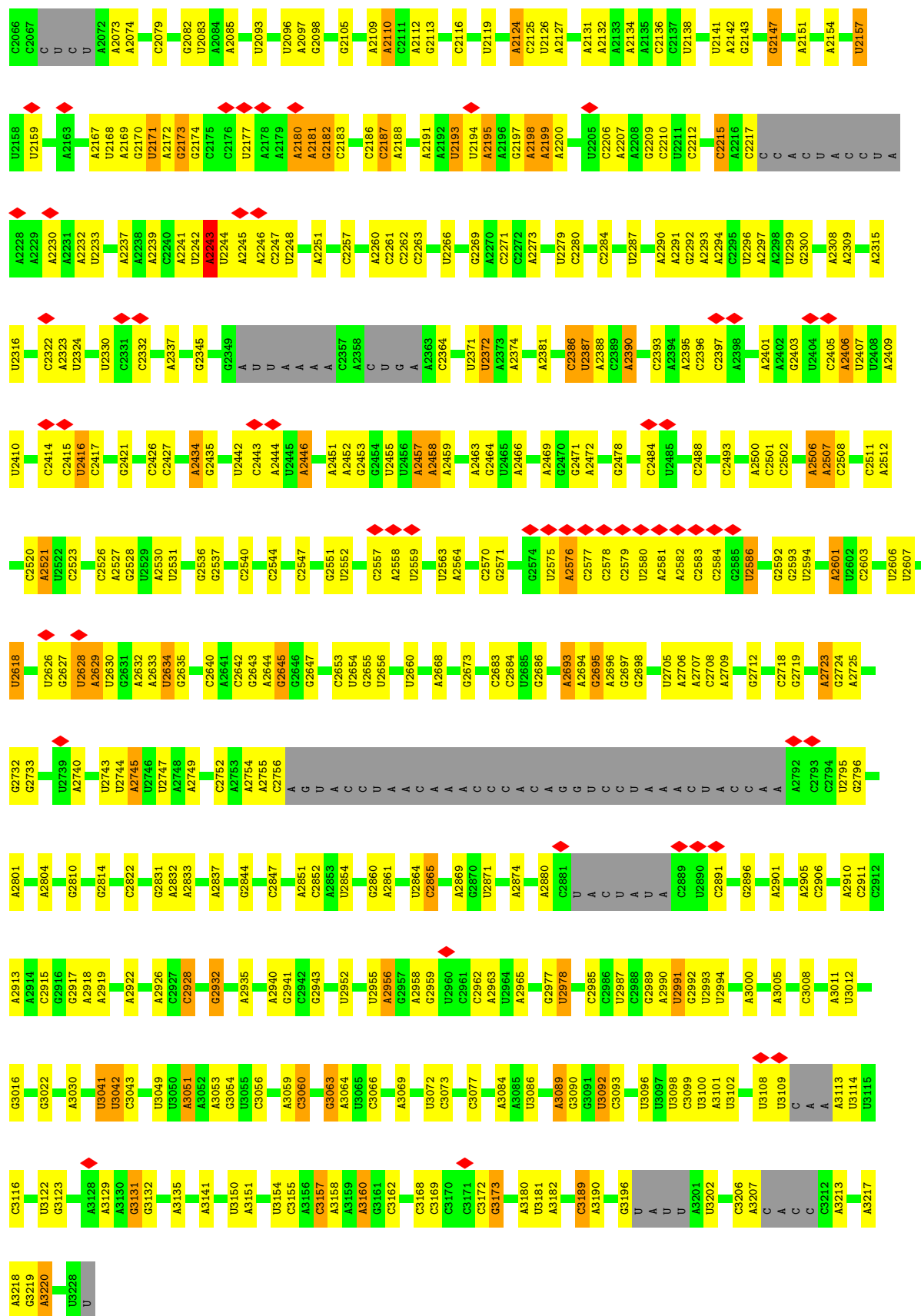


- Molecule 53: Acyl carrier protein, mitochondrial

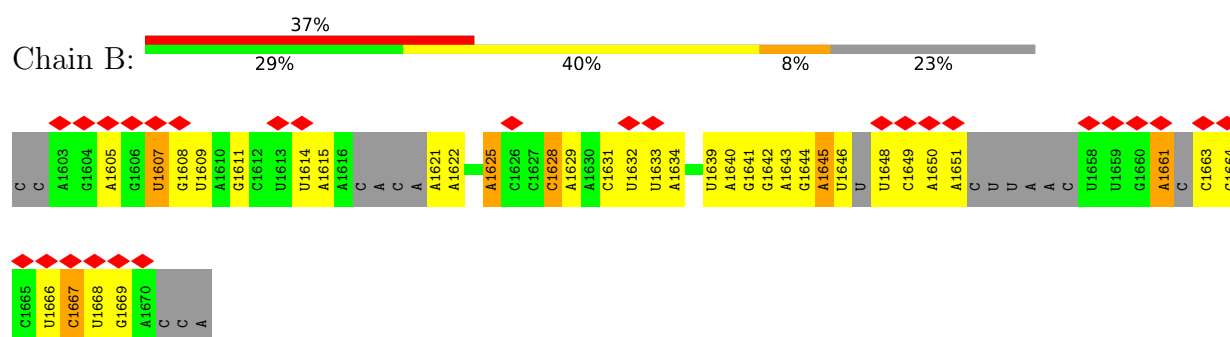


- Molecule 54: 16S rRNA

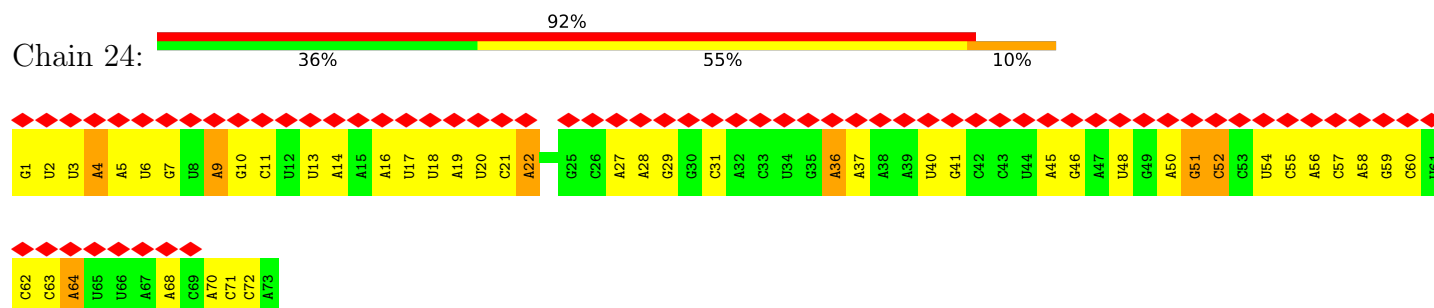




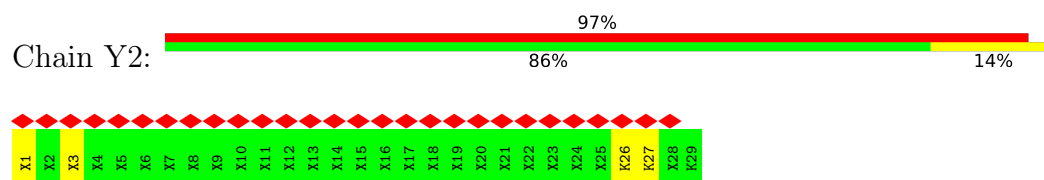
- Molecule 55: mt-tRNAVal



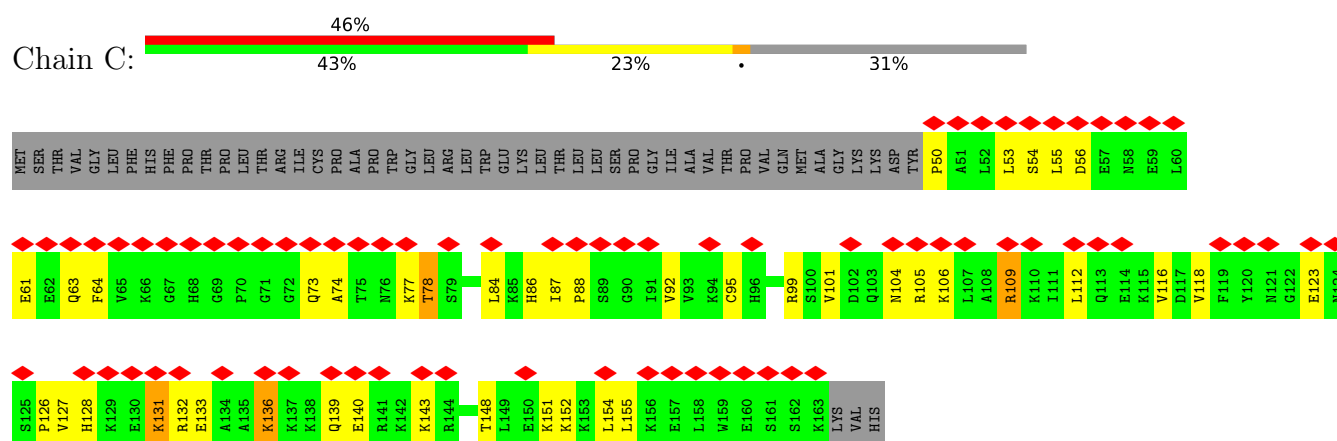
- Molecule 56: mt-tRNA



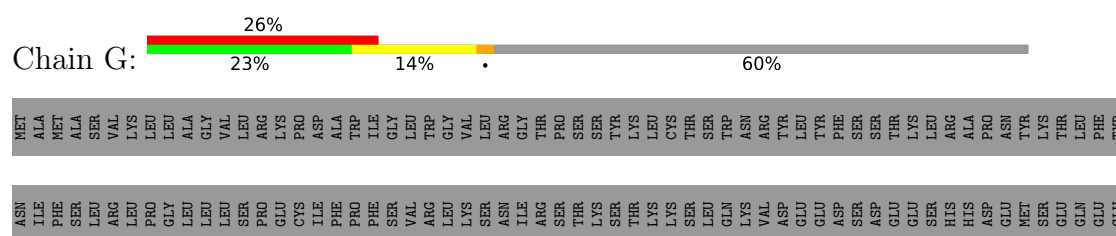
- Molecule 57: nascent chain

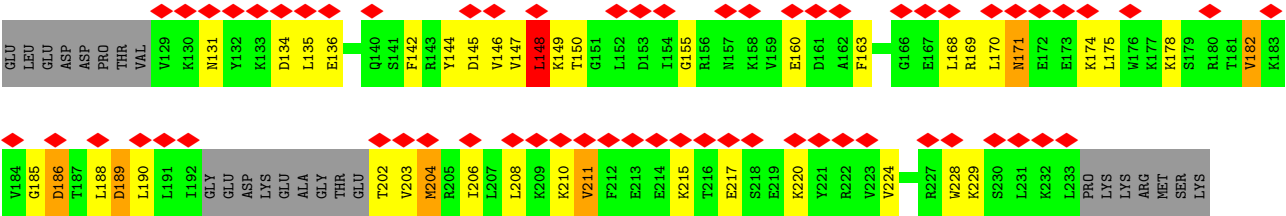


- Molecule 58: Probable peptide chain release factor C12orf65, mitochondrial



- Molecule 59: Mitochondrial transcription rescue factor 1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	48245	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.675	Depositor
Minimum map value	-0.378	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.11	Depositor
Map size (Å)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PNS, ZN, MG, MEQ

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	D	0.66	0/1879	0.78	1/2527 (0.0%)
2	E	0.67	0/2465	0.71	0/3344
3	F	0.70	0/2071	0.68	0/2817
4	H	0.53	0/798	0.73	0/1073
5	I	0.44	0/1308	0.78	1/1761 (0.1%)
6	J	0.37	0/1077	0.81	2/1452 (0.1%)
7	K	0.70	0/1495	0.68	1/2029 (0.0%)
8	L	0.64	0/904	0.80	0/1218
9	M	0.68	0/2359	0.72	0/3185
10	N	0.63	0/1697	0.70	0/2281
11	O	0.66	0/1269	0.71	0/1708
12	P	0.55	0/1173	0.68	0/1588
13	Q	0.59	0/1846	0.73	2/2487 (0.1%)
14	R	0.73	0/1174	0.65	0/1572
15	S	0.70	0/1276	0.73	0/1729
16	T	0.68	1/1402 (0.1%)	0.69	0/1886
17	U	0.62	0/1247	0.84	1/1689 (0.1%)
18	V	0.50	0/1666	0.72	4/2260 (0.2%)
19	W	0.70	0/881	0.62	0/1188
20	X	0.57	0/2090	0.68	0/2825
21	Y	0.66	1/1552 (0.1%)	0.66	0/2079
22	Z	0.64	0/1003	0.69	0/1354
23	0	0.62	0/895	0.73	0/1201
24	1	0.61	0/438	0.71	0/583
25	2	0.82	0/373	0.76	0/496
26	3	0.76	0/852	0.71	0/1136
27	5	0.56	0/3250	0.71	0/4429
28	6	0.55	1/2726 (0.0%)	0.71	2/3715 (0.1%)
29	7	0.51	0/2391	0.70	0/3234
30	8	0.38	0/909	0.96	9/1227 (0.7%)
31	9	0.59	0/972	0.72	0/1306
32	a	0.55	0/709	0.65	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	b	0.65	0/1202	0.73	0/1626
34	c	0.55	0/2264	0.67	0/3059
35	d	0.45	0/1790	0.67	0/2423
36	e	0.37	0/1797	0.71	0/2422
37	f	0.43	0/931	0.68	0/1259
38	g	0.66	0/1102	0.75	0/1503
39	h	0.44	0/847	0.68	0/1150
40	i	0.77	0/849	0.73	0/1135
41	j	0.54	0/698	0.63	0/940
42	k	0.43	0/635	0.68	0/855
43	l	0.48	0/226	0.56	0/299
44	m	0.37	0/379	0.88	0/510
45	o	0.68	0/792	0.74	0/1064
46	p	0.44	0/1071	0.64	0/1433
47	q	0.45	0/1107	0.60	0/1498
48	r	0.63	0/1238	0.66	0/1676
49	s	0.62	0/3114	0.68	0/4225
51	u	0.48	0/949	0.69	0/1281
52	v	0.42	0/597	0.74	0/796
53	w	0.29	0/647	0.70	0/871
54	A	0.77	0/34613	0.60	6/53854 (0.0%)
55	B	0.36	0/1328	0.53	0/2056
56	24	0.33	0/1731	0.56	0/2693
57	Y2	0.51	0/25	0.83	0/27
58	C	0.45	0/929	0.90	1/1235 (0.1%)
59	G	0.50	0/818	1.18	4/1090 (0.4%)
All	All	0.64	3/107826 (0.0%)	0.68	34/153322 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
15	S	0	1
18	V	0	1
27	5	0	2
30	8	0	3
48	r	0	2
49	s	0	1
57	Y2	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
59	G	0	2
All	All	0	14

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	6	28	ARG	C-N	-11.02	1.18	1.33
16	T	58	VAL	C-N	-6.08	1.15	1.33
21	Y	195	ASN	CA-C	-5.75	1.44	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	102	VAL	N-CA-C	-9.60	103.98	113.20
59	G	145	ASP	N-CA-C	-8.59	104.83	114.62
59	G	189	ASP	CA-C-N	8.28	137.36	121.54
59	G	189	ASP	C-N-CA	8.28	137.36	121.54
17	U	118	PRO	N-CA-CB	8.10	111.75	103.25
30	8	183	PRO	N-CA-CB	7.62	111.25	103.25
58	C	131	LYS	N-CA-C	-7.57	105.99	114.62
30	8	186	GLN	CA-C-N	7.36	127.97	120.38
30	8	186	GLN	C-N-CA	7.36	127.97	120.38
30	8	185	TYR	N-CA-C	7.28	117.59	108.19
7	K	137	ILE	N-CA-C	-7.07	105.89	112.96
6	J	134	ASP	CA-C-N	7.06	124.69	120.24
6	J	134	ASP	C-N-CA	7.06	124.69	120.24
59	G	211	VAL	N-CA-C	-6.88	106.60	113.20
30	8	187	PRO	N-CA-CB	6.84	109.71	103.08
18	V	160	PRO	N-CA-CB	6.07	109.62	103.25
30	8	188	PRO	N-CA-CB	6.02	109.57	103.25
28	6	254	TYR	CA-C-N	5.93	132.78	122.28
28	6	254	TYR	C-N-CA	5.93	132.78	122.28
54	A	1823	A	P-O3'-C3'	5.74	128.81	120.20
54	A	2243	A	C2'-C3'-O3'	5.72	118.07	109.50
18	V	167	PRO	N-CA-CB	5.69	109.22	103.25
30	8	97	LYS	CA-CB-CG	5.50	125.10	114.10
54	A	2507	A	C2'-C3'-O3'	5.46	121.89	113.70
54	A	2243	A	P-O3'-C3'	5.45	128.38	120.20
18	V	166	VAL	CA-C-N	5.44	126.64	119.84
18	V	166	VAL	C-N-CA	5.44	126.64	119.84
13	Q	87	THR	CA-C-N	5.40	127.90	120.39
13	Q	87	THR	C-N-CA	5.40	127.90	120.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	A	3092	U	C4'-C3'-O3'	5.32	120.98	113.00
30	8	185	TYR	CA-C-N	5.27	134.66	121.80
30	8	185	TYR	C-N-CA	5.27	134.66	121.80
1	D	207	ILE	N-CA-C	5.26	120.28	109.34
54	A	2457	A	P-O3'-C3'	5.21	128.01	120.20

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	5	216	GLU	Peptide
27	5	217	SER	Peptide
30	8	179	THR	Peptide
30	8	184	ASN	Peptide
30	8	186	GLN	Peptide
1	D	206	TYR	Peptide
59	G	148	LEU	Peptide
59	G	211	VAL	Peptide
15	S	101	PHE	Peptide
18	V	100	LYS	Peptide
57	Y2	27	LYS	Peptide
48	r	54	THR	Peptide
48	r	67	SER	Peptide
49	s	270	LYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1842	0	1896	34	0
2	E	2396	0	2402	28	0
3	F	2013	0	2044	26	0
4	H	784	0	832	5	0
5	I	1283	0	1369	26	0
6	J	1061	0	1141	24	0
7	K	1451	0	1448	20	0
8	L	889	0	941	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	M	2305	0	2378	30	0
10	N	1654	0	1681	22	0
11	O	1245	0	1283	19	0
12	P	1148	0	1148	30	0
13	Q	1805	0	1841	25	0
14	R	1153	0	1214	19	0
15	S	1251	0	1322	19	0
16	T	1368	0	1409	23	0
17	U	1218	0	1186	24	0
18	V	1624	0	1606	20	0
19	W	859	0	888	11	0
20	X	2035	0	2054	21	0
21	Y	1517	0	1561	16	0
22	Z	978	0	1030	16	0
23	0	880	0	902	16	0
24	1	433	0	475	12	0
25	2	367	0	393	3	0
26	3	831	0	883	16	0
27	5	3156	0	3138	45	0
28	6	2640	0	2464	41	0
29	7	2334	0	2343	26	0
30	8	890	0	864	18	0
31	9	947	0	949	11	0
32	a	686	0	658	7	0
33	b	1178	0	1180	21	0
34	c	2217	0	2220	25	0
35	d	1741	0	1727	23	0
36	e	1762	0	1767	36	0
37	f	915	0	917	13	0
38	g	1067	0	1056	12	0
39	h	827	0	806	11	0
40	i	827	0	857	14	0
41	j	684	0	673	10	0
42	k	627	0	636	14	0
43	l	221	0	227	4	0
44	m	372	0	387	10	0
45	o	771	0	775	13	0
46	p	1058	0	1083	16	0
47	q	1076	0	1049	16	0
48	r	1203	0	1220	17	0
49	s	3036	0	3022	43	0
50	t	140	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	u	927	0	921	21	0
52	v	588	0	604	19	0
53	w	638	0	636	13	0
54	A	30945	0	15722	152	0
55	B	1191	0	607	13	0
56	24	1547	0	787	11	0
57	Y2	157	0	80	2	0
58	C	928	0	974	23	0
59	G	809	0	869	17	0
60	A	89	0	0	0	0
60	D	1	0	0	0	0
60	W	1	0	0	0	0
60	g	1	0	0	0	0
61	0	1	0	0	0	0
61	r	1	0	0	0	0
62	v	21	0	21	4	0
All	All	102610	0	86596	1018	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (1018) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:P:39:VAL:HG12	12:P:41:ASN:H	1.51	0.74
42:k:64:VAL:HB	42:k:76:MET:HB2	1.72	0.70
9:M:246:ASP:OD1	9:M:246:ASP:N	2.26	0.69
12:P:118:SER:OG	12:P:121:ASN:ND2	2.27	0.68
6:J:89:TYR:HA	6:J:92:LYS:HE2	1.76	0.67
14:R:54:THR:HG21	15:S:172:MET:H	1.57	0.67
54:A:1747:G:N2	54:A:1750:G:O2'	2.27	0.67
54:A:3089:A:H5''	56:24:71:C:H5''	1.77	0.67
29:7:286:LEU:HB2	29:7:294:ILE:HG13	1.76	0.67
17:U:28:LEU:H	21:Y:114:THR:HG22	1.59	0.67
22:Z:99:VAL:O	41:j:76:ARG:NH2	2.28	0.66
6:J:110:GLY:HA3	6:J:153:ILE:HG13	1.76	0.66
59:G:147:VAL:HG13	59:G:188:LEU:HD21	1.76	0.66
49:s:143:ARG:HH21	49:s:413:PHE:HB3	1.62	0.65
52:v:16:LEU:HD23	52:v:62:LEU:HD13	1.77	0.65
12:P:138:GLU:OE1	28:6:136:ARG:NH2	2.30	0.65
30:8:139:MET:HG2	36:e:275:PHE:HA	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:3:SER:O	34:c:302:ARG:NH1	2.30	0.64
12:P:85:ARG:NH1	12:P:125:CYS:SG	2.71	0.64
2:E:220:LYS:NZ	54:A:3160:A:OP1	2.31	0.64
30:8:134:ASP:HA	30:8:137:ARG:HH11	1.63	0.64
1:D:154:THR:H	1:D:157:MET:HE3	1.63	0.64
16:T:69:ARG:NH1	35:d:228:PHE:O	2.31	0.64
3:F:103:GLN:HE22	3:F:249:ASN:HB2	1.63	0.64
45:o:65:VAL:HG12	45:o:68:ARG:HH12	1.63	0.64
2:E:207:THR:HG23	2:E:298:LYS:HB3	1.79	0.64
34:c:73:GLN:HG3	34:c:85:LEU:HD11	1.78	0.64
1:D:172:MET:HE3	1:D:173:ALA:H	1.63	0.63
9:M:202:LYS:HD2	9:M:263:ARG:HE	1.63	0.63
6:J:25:ARG:HA	6:J:65:PRO:HA	1.80	0.63
22:Z:131:GLU:HA	22:Z:134:MET:HB2	1.81	0.63
2:E:150:LYS:HD2	2:E:296:LEU:HD11	1.79	0.63
10:N:188:LYS:NZ	10:N:198:MET:SD	2.69	0.63
33:b:45:GLU:OE2	33:b:49:ARG:NH2	2.31	0.63
47:q:89:GLU:HG2	47:q:93:TYR:HB2	1.81	0.63
3:F:223:HIS:HA	3:F:226:MET:HE3	1.80	0.63
30:8:100:GLU:HB3	30:8:101:ARG:HD3	1.80	0.63
51:u:110:CYS:HA	52:v:26:THR:HB	1.81	0.63
1:D:228:LEU:HD11	1:D:234:MET:HE3	1.81	0.63
2:E:269:TYR:HB3	2:E:304:LEU:HD21	1.81	0.63
56:24:29:G:N2	56:24:37:A:N1	2.47	0.63
51:u:131:SER:OG	51:u:132:THR:N	2.31	0.62
5:I:98:VAL:HG21	5:I:146:LEU:HD11	1.80	0.62
52:v:46:GLU:HB2	52:v:51:ARG:HE	1.64	0.62
52:v:6:ARG:NH1	62:v:101:PNS:O23	2.33	0.62
5:I:83:ARG:HA	5:I:134:PHE:HE2	1.64	0.62
49:s:257:VAL:HG12	49:s:259:ILE:H	1.64	0.62
15:S:177:ARG:NH2	54:A:1853:A:OP2	2.33	0.62
5:I:80:ARG:HA	5:I:83:ARG:HB2	1.80	0.62
46:p:78:ILE:HG12	46:p:101:VAL:HG22	1.81	0.62
21:Y:95:ASN:OD1	21:Y:149:ARG:NH1	2.33	0.62
36:e:64:THR:HG22	36:e:66:LEU:H	1.65	0.62
14:R:36:ASN:OD1	14:R:36:ASN:N	2.32	0.62
49:s:251:VAL:O	49:s:373:GLN:NE2	2.32	0.61
54:A:2195:A:H1'	54:A:2215:C:H1'	1.82	0.61
36:e:65:PRO:HA	36:e:68:GLU:HB2	1.81	0.61
55:B:1648:U:H3	55:B:1661:A:H61	1.47	0.61
1:D:124:GLU:OE2	1:D:165:ASN:ND2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:b:35:ARG:HG3	45:o:101:TRP:HB2	1.82	0.61
53:w:100:VAL:HA	53:w:141:PRO:HG2	1.82	0.61
1:D:194:ASN:HD22	1:D:247:VAL:HG22	1.65	0.61
7:K:8:PRO:HG2	34:c:295:GLU:HG3	1.82	0.61
22:Z:101:LYS:HE3	41:j:80:LEU:HD22	1.82	0.61
26:3:183:ARG:NH1	28:6:355:LYS:O	2.32	0.61
17:U:38:ASP:OD1	17:U:98:GLN:NE2	2.33	0.61
56:24:6:U:H3	56:24:64:A:H61	1.47	0.61
32:a:104:GLU:HB2	32:a:107:PRO:HD2	1.81	0.60
33:b:27:GLN:HE21	33:b:80:LEU:HA	1.64	0.60
47:q:41:ASP:OD1	47:q:41:ASP:N	2.34	0.60
21:Y:193:ARG:NH2	54:A:1706:C:OP1	2.34	0.60
58:C:101:VAL:HA	58:C:104:ASN:HB2	1.82	0.60
16:T:157:ARG:HB2	16:T:167:MET:HE3	1.82	0.60
27:5:49:VAL:HA	27:5:52:ILE:HD12	1.82	0.60
56:24:70:A:H5'	56:24:71:C:H5'	1.82	0.60
31:9:16:ASP:O	31:9:25:ARG:NH1	2.34	0.60
54:A:2191:A:N6	54:A:2198:A:OP2	2.33	0.60
28:6:360:ARG:NH1	54:A:2869:A:N7	2.45	0.60
53:w:100:VAL:O	53:w:142:GLN:NE2	2.34	0.60
18:V:55:TYR:O	18:V:145:ARG:NH2	2.34	0.60
58:C:63:GLN:HE21	58:C:64:PHE:H	1.48	0.60
8:L:118:ARG:NH2	51:u:188:TYR:O	2.29	0.60
25:2:69:ARG:NH1	54:A:1916:G:OP1	2.35	0.60
30:8:173:LYS:NZ	37:f:175:GLN:O	2.35	0.60
36:e:200:MET:HA	36:e:241:GLY:HA2	1.83	0.60
3:F:137:ARG:NH2	54:A:2932:G:OP1	2.34	0.60
36:e:151:ARG:NH1	36:e:254:TRP:O	2.35	0.60
12:P:77:PHE:O	12:P:97:GLN:NE2	2.35	0.59
18:V:104:TYR:HD1	18:V:105:ARG:H	1.50	0.59
41:j:102:GLN:NE2	41:j:106:GLU:OE2	2.35	0.59
56:24:36:A:O2'	59:G:131:ASN:ND2	2.35	0.59
3:F:92:ARG:NH2	54:A:1878:U:O3'	2.36	0.59
29:7:112:PRO:HB2	29:7:267:PRO:HG2	1.85	0.59
2:E:236:THR:HG22	2:E:239:ARG:HD3	1.85	0.59
14:R:96:GLU:OE2	41:j:28:ARG:NH1	2.33	0.59
40:i:115:ARG:NH1	54:A:2010:U:OP2	2.35	0.59
56:24:72:C:OP2	58:C:99:ARG:NH1	2.36	0.59
3:F:252:SER:O	3:F:256:HIS:ND1	2.35	0.59
8:L:141:ALA:O	51:u:197:ARG:NH2	2.34	0.59
29:7:196:LYS:HA	29:7:199:LEU:HD12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:p:56:ASP:HB2	46:p:60:ARG:HE	1.67	0.59
54:A:1777:A:N6	54:A:1780:U:OP2	2.36	0.59
49:s:304:ASP:N	49:s:304:ASP:OD1	2.36	0.59
1:D:108:ASP:OD2	1:D:149:ARG:NH1	2.36	0.58
1:D:184:LEU:HD13	1:D:226:ILE:HD11	1.84	0.58
6:J:84:GLN:NE2	6:J:123:ILE:O	2.36	0.58
11:O:25:ARG:NH2	11:O:51:GLU:OE2	2.34	0.58
12:P:66:ARG:NH2	54:A:2874:A:O2'	2.36	0.58
5:I:151:ASN:OD1	42:k:31:ARG:NH1	2.36	0.58
12:P:51:ARG:NH1	28:6:221:LEU:O	2.36	0.58
18:V:199:MET:HE3	18:V:204:ILE:HB	1.85	0.58
36:e:53:LEU:HD11	36:e:238:LEU:HG	1.86	0.58
3:F:271:ASP:OD1	3:F:272:LYS:NZ	2.37	0.58
11:O:106:ARG:NH2	11:O:124:GLU:OE2	2.36	0.58
26:3:113:ARG:NH2	54:A:1750:G:OP2	2.36	0.58
28:6:221:LEU:HD12	28:6:267:ARG:HG3	1.84	0.58
28:6:160:ASP:OD1	28:6:267:ARG:NH2	2.37	0.58
36:e:88:GLU:HB3	36:e:92:LEU:HD12	1.84	0.58
37:f:48:TYR:N	54:A:2065:A:OP1	2.36	0.58
33:b:72:VAL:HG13	33:b:90:HIS:HB2	1.86	0.58
54:A:2112:A:HO2'	54:A:2943:G:HO2'	1.51	0.58
1:D:111:ARG:NH2	1:D:179:GLY:O	2.35	0.58
46:p:182:ASN:OD1	46:p:185:ARG:NH1	2.37	0.58
14:R:114:LYS:HD2	32:a:44:ASN:HB3	1.85	0.58
15:S:120:LEU:HB3	15:S:122:LEU:HD12	1.86	0.58
44:m:77:MET:HG2	44:m:78:PRO:HD2	1.86	0.58
54:A:2093:U:O2	54:A:2266:U:O2'	2.21	0.58
10:N:111:ARG:NH1	54:A:2956:A:O2'	2.37	0.57
17:U:64:PRO:HB2	17:U:100:ALA:HB3	1.85	0.57
37:f:99:ASP:OD2	44:m:67:ARG:NH1	2.37	0.57
48:r:188:SER:HB3	54:A:2243:A:H5''	1.86	0.57
56:24:11:C:H42	56:24:22:A:H61	1.52	0.57
10:N:191:SER:OG	10:N:192:ARG:N	2.38	0.57
35:d:208:VAL:HG13	35:d:252:LEU:HB2	1.86	0.57
47:q:138:GLN:NE2	47:q:142:ASN:OD1	2.37	0.57
16:T:144:GLU:HG3	16:T:177:LYS:HE2	1.87	0.57
40:i:46:ARG:NH2	54:A:2279:U:OP2	2.35	0.57
49:s:81:ARG:NH1	54:A:2442:U:OP1	2.36	0.57
54:A:3063:G:O2'	54:A:3066:C:OP2	2.19	0.57
6:J:21:ARG:NH1	54:A:2169:A:OP1	2.32	0.57
30:8:164:ARG:HD2	37:f:81:ASN:HD21	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:278:LYS:NZ	54:A:2634:U:OP2	2.35	0.57
10:N:218:ILE:HG23	10:N:223:MET:HB2	1.87	0.57
6:J:145:ILE:HG13	6:J:155:VAL:HG21	1.85	0.57
3:F:123:GLY:HA3	3:F:142:ARG:HG2	1.87	0.57
12:P:178:ILE:O	28:6:346:ARG:NH2	2.37	0.57
17:U:17:LEU:HD11	31:9:136:LEU:HD22	1.85	0.57
27:5:299:LEU:HG	27:5:301:PRO:HD2	1.85	0.57
51:u:200:ASP:N	51:u:200:ASP:OD1	2.38	0.57
20:X:238:LEU:HD23	31:9:105:LYS:HE3	1.87	0.57
34:c:251:SER:OG	34:c:252:ALA:N	2.38	0.57
16:T:57:ILE:O	35:d:227:ARG:NH1	2.38	0.57
18:V:124:ASP:N	18:V:124:ASP:OD1	2.37	0.57
27:5:310:ARG:HA	27:5:313:MET:HE2	1.87	0.57
39:h:93:ASP:HB3	39:h:96:LEU:HB2	1.87	0.57
58:C:56:ASP:OD1	58:C:56:ASP:N	2.37	0.57
7:K:119:ARG:NH1	54:A:2705:U:OP2	2.37	0.56
9:M:116:ILE:HB	9:M:154:ILE:HG23	1.87	0.56
14:R:99:ARG:NH2	54:A:2248:U:OP1	2.37	0.56
15:S:161:ILE:HD13	33:b:17:ASN:HB3	1.87	0.56
27:5:223:ARG:NH1	54:A:2410:U:OP1	2.38	0.56
20:X:17:ARG:HH22	47:q:43:GLU:HG3	1.71	0.56
1:D:213:CYS:HB3	1:D:246:ARG:HB3	1.86	0.56
2:E:150:LYS:HB2	2:E:296:LEU:HD21	1.87	0.56
12:P:88:HIS:O	12:P:119:THR:OG1	2.22	0.56
24:1:55:LEU:HB2	47:q:128:MET:HE1	1.88	0.56
26:3:108:LYS:NZ	54:A:1745:U:O4	2.38	0.56
30:8:173:LYS:H	37:f:184:LEU:HB2	1.69	0.56
9:M:264:GLN:NE2	9:M:267:PHE:O	2.38	0.56
13:Q:129:LYS:NZ	51:u:121:THR:O	2.37	0.56
20:X:64:ASP:OD1	20:X:64:ASP:N	2.39	0.56
34:c:148:MET:HG2	34:c:153:ILE:HG13	1.87	0.56
41:j:63:GLN:OE1	41:j:66:ARG:NH2	2.39	0.56
49:s:214:GLU:HA	49:s:228:ASP:HA	1.87	0.56
3:F:226:MET:SD	47:q:26:ARG:NH1	2.79	0.56
54:A:2576:A:H62	58:C:136:LYS:HD3	1.69	0.56
2:E:276:ILE:HD11	2:E:332:LEU:HD12	1.87	0.56
6:J:98:GLU:HG3	6:J:99:LYS:HG2	1.88	0.56
9:M:185:ASP:OD1	9:M:185:ASP:N	2.38	0.56
10:N:168:GLU:OE2	43:l:128:ARG:NH1	2.39	0.56
28:6:222:ASP:OD2	28:6:267:ARG:NH1	2.36	0.56
12:P:63:ARG:NH1	19:W:137:LYS:O	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Q:231:LYS:NZ	54:A:3154:U:OP1	2.38	0.56
52:v:43:GLN:OE1	62:v:101:PNS:N41	2.37	0.56
1:D:199:GLU:HB2	1:D:202:ARG:HB2	1.88	0.56
18:V:102:MET:SD	18:V:102:MET:N	2.79	0.56
49:s:80:LEU:O	49:s:84:THR:OG1	2.23	0.56
58:C:61:GLU:HB2	58:C:87:ILE:HD11	1.87	0.56
5:I:164:MET:HA	5:I:167:ILE:HD12	1.88	0.56
8:L:43:ASN:HD22	8:L:117:THR:HB	1.70	0.56
36:e:199:ASN:HB2	36:e:242:ASP:HB2	1.88	0.56
45:o:54:MET:HB3	45:o:58:GLN:HB2	1.88	0.56
58:C:84:LEU:HD13	58:C:109[A]:ARG:HH21	1.71	0.56
58:C:84:LEU:HD13	58:C:109[B]:ARG:HH21	1.71	0.56
6:J:50:CYS:O	6:J:54:ASN:ND2	2.39	0.55
29:7:153:VAL:HG13	29:7:205:ASP:HB2	1.88	0.55
49:s:376:THR:HG21	49:s:387:ASN:HD21	1.70	0.55
12:P:52:ASN:HB3	12:P:55:ASN:HB2	1.87	0.55
5:I:37:ARG:HH12	10:N:247:MET:HE3	1.71	0.55
24:1:19:ARG:HB2	24:1:62:ILE:HD11	1.89	0.55
30:8:117:LEU:HD23	36:e:73:LEU:HD13	1.87	0.55
40:i:73:LEU:HD11	47:q:31:PRO:HG3	1.89	0.55
10:N:208:ASN:O	10:N:210:GLN:NE2	2.39	0.55
16:T:72:GLU:HG2	16:T:179:VAL:HG22	1.88	0.55
17:U:78:LYS:NZ	54:A:2364:C:OP1	2.36	0.55
28:6:142:THR:OG1	28:6:143:CYS:N	2.38	0.55
35:d:118:SER:O	35:d:118:SER:OG	2.25	0.55
36:e:99:ALA:HA	36:e:102:LYS:HB2	1.88	0.55
8:L:111:ASN:OD1	8:L:111:ASN:N	2.39	0.55
28:6:222:ASP:OD1	28:6:222:ASP:N	2.40	0.55
31:9:100:ILE:O	31:9:104:PHE:N	2.40	0.55
26:3:106:THR:HG22	26:3:163:THR:H	1.71	0.55
1:D:202:ARG:O	54:A:2521:A:N6	2.40	0.55
44:m:56:LEU:HA	44:m:75:LEU:HB2	1.89	0.55
27:5:33:TRP:O	27:5:39:ARG:NH2	2.40	0.55
34:c:31:VAL:N	54:A:1773:A:OP1	2.39	0.55
34:c:244:GLU:OE2	34:c:248:ARG:NH1	2.40	0.55
2:E:138:CYS:SG	2:E:139:ASN:N	2.80	0.54
27:5:93:LEU:HB3	27:5:270:ILE:HD11	1.88	0.54
54:A:2232:A:N6	54:A:2978:U:OP1	2.40	0.54
1:D:132:ASP:OD2	1:D:135:ARG:NH1	2.38	0.54
22:Z:82:GLU:OE1	22:Z:115:HIS:NE2	2.37	0.54
53:w:138:LEU:HD13	53:w:144:ILE:HG12	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:22:ASP:O	7:K:147:GLN:NE2	2.40	0.54
9:M:131:PRO:HG2	9:M:185:ASP:HB3	1.89	0.54
12:P:54:ARG:HH11	12:P:58:LEU:HD21	1.73	0.54
30:8:146:ALA:O	30:8:150:LEU:N	2.39	0.54
40:i:71:LYS:HD2	40:i:82:GLY:HA3	1.88	0.54
2:E:344:SER:HB3	13:Q:102:ARG:HH12	1.73	0.54
26:3:131:LYS:O	26:3:136:LYS:NZ	2.41	0.54
42:k:16:VAL:HG22	42:k:66:VAL:HG13	1.89	0.54
56:24:28:A:H2'	56:24:29:G:H8	1.73	0.54
6:J:112:VAL:HG13	6:J:116:HIS:HB3	1.89	0.54
10:N:177:ASP:O	10:N:181:HIS:ND1	2.40	0.54
14:R:48:ARG:NH2	54:A:1844:A:OP2	2.41	0.54
29:7:67:VAL:HG13	29:7:79:PHE:HB2	1.88	0.54
43:l:114:SER:OG	43:l:115:ARG:N	2.39	0.54
59:G:136:GLU:H	59:G:224:VAL:HA	1.72	0.54
33:b:26:LEU:HD13	33:b:61:VAL:HG11	1.89	0.54
37:f:178:LEU:HB3	37:f:182:VAL:HG23	1.89	0.54
42:k:78:GLY:HA2	42:k:81:LEU:HB2	1.89	0.54
6:J:136:PRO:HG2	6:J:139:SER:HB3	1.88	0.54
7:K:63:ARG:NH1	7:K:130:ASP:OD1	2.41	0.54
9:M:133:LYS:NZ	54:A:1889:C:OP1	2.38	0.54
10:N:114:ASP:H	10:N:118:MET:HE3	1.72	0.54
11:O:67:ASP:N	11:O:67:ASP:OD1	2.40	0.54
20:X:142:ASP:OD1	20:X:142:ASP:N	2.38	0.54
49:s:160:ARG:NH1	54:A:2409:A:OP1	2.35	0.54
9:M:46:GLY:HA2	9:M:49:CYS:HA	1.90	0.54
9:M:50:GLY:O	40:i:126:LYS:NZ	2.38	0.54
15:S:139:ASP:OD1	34:c:310:ASN:ND2	2.40	0.54
16:T:52:GLU:OE1	16:T:78:ARG:NH2	2.35	0.54
27:5:341:VAL:HG22	27:5:358:GLN:HG3	1.90	0.54
2:E:129:VAL:O	2:E:190:GLY:N	2.40	0.54
3:F:241:ASN:OD1	3:F:256:HIS:NE2	2.27	0.54
39:h:88:ASP:OD1	39:h:124:ARG:NH1	2.41	0.54
49:s:211:VAL:HG22	49:s:230:ARG:HG2	1.89	0.54
52:v:7:GLU:HG3	52:v:11:SER:HB2	1.88	0.54
55:B:1607:U:H3	55:B:1664:G:H1	1.55	0.54
7:K:21:LEU:HG	7:K:145:LEU:HB2	1.90	0.54
1:D:71:LYS:NZ	54:A:2386:C:OP2	2.36	0.53
3:F:181:LYS:NZ	3:F:257:GLN:O	2.36	0.53
23:0:106:ASN:OD1	23:0:106:ASN:N	2.41	0.53
27:5:125:LYS:HG2	27:5:371:LYS:HG2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:7:173:PRO:O	29:7:176:SER:OG	2.25	0.53
30:8:165:ASP:OD2	36:e:185:ARG:NH2	2.40	0.53
1:D:122:PHE:HE2	1:D:165:ASN:HD22	1.55	0.53
8:L:35:MET:O	8:L:37:ARG:NH2	2.41	0.53
19:W:101:LYS:NZ	54:A:2064:A:OP1	2.39	0.53
28:6:178:ALA:HA	28:6:184:LEU:HA	1.90	0.53
29:7:115:MET:HB2	29:7:270:PRO:HB3	1.90	0.53
35:d:119:GLN:O	35:d:123:ARG:NH1	2.41	0.53
37:f:110:VAL:HG12	37:f:174:ILE:HD12	1.90	0.53
51:u:150:LYS:HD3	51:u:151:CYS:H	1.73	0.53
54:A:1964:U:H4'	54:A:2434:A:H8	1.73	0.53
54:A:2537:G:O2'	54:A:2634:U:OP2	2.26	0.53
54:A:2618:U:O4	54:A:3043:C:N4	2.37	0.53
29:7:217:GLU:HB2	29:7:256:ARG:HB3	1.91	0.53
1:D:105:ARG:NH2	54:A:2403:G:OP2	2.40	0.53
54:A:2822:C:O2'	54:A:2915:C:OP2	2.26	0.53
58:C:136:LYS:HA	58:C:139:GLN:HE21	1.72	0.53
59:G:148:LEU:O	59:G:150:THR:N	2.41	0.53
3:F:107:LYS:HG2	40:i:74:ILE:HG22	1.91	0.53
47:q:144:GLU:O	47:q:148:ALA:N	2.32	0.53
4:H:85:ASP:OD2	54:A:2796:G:O2'	2.25	0.53
13:Q:87:THR:HG21	13:Q:91:LYS:HD2	1.91	0.53
20:X:102:LYS:O	54:A:2745:A:O2'	2.25	0.53
28:6:149:GLN:NE2	28:6:166:THR:OG1	2.40	0.53
54:A:2643:G:O2'	54:A:2645:G:OP2	2.22	0.53
19:W:74:ARG:HE	54:A:2065:A:H5'	1.73	0.53
28:6:371:ASP:OD1	28:6:371:ASP:N	2.37	0.53
59:G:144:TYR:OH	59:G:169:ARG:O	2.19	0.53
7:K:13:THR:OG1	33:b:129:GLN:NE2	2.42	0.53
28:6:219:THR:OG1	28:6:220:SER:N	2.42	0.53
34:c:87:LEU:HD21	34:c:204:GLN:HB2	1.91	0.53
48:r:71:PRO:HD2	48:r:107:LEU:HD23	1.91	0.53
54:A:2387:U:O2'	54:A:2406:A:N6	2.40	0.53
8:L:35:MET:HE2	54:A:2472:A:H5''	1.91	0.52
11:O:96:ARG:NH1	11:O:127:GLY:O	2.41	0.52
11:O:129:CYS:SG	23:0:156:THR:OG1	2.67	0.52
21:Y:225:ASN:HD21	54:A:1683:C:H41	1.57	0.52
54:A:2032:G:O2'	54:A:2865:C:O2	2.23	0.52
27:5:343:GLN:NE2	27:5:417:LEU:O	2.41	0.52
13:Q:232:ARG:NH1	54:A:2466:A:OP1	2.42	0.52
19:W:67:ILE:HG21	19:W:131:VAL:HG11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:8:154:SER:OG	36:e:230:LYS:NZ	2.39	0.52
32:a:44:ASN:ND2	33:b:135:ASN:OD1	2.43	0.52
49:s:103:ASP:OD1	49:s:325:ARG:NH1	2.40	0.52
54:A:3011:A:O2'	54:A:3173:G:N2	2.43	0.52
26:3:98:SER:HB2	26:3:105:LYS:HE3	1.91	0.52
30:8:154:SER:HB3	30:8:157:LEU:HD13	1.91	0.52
54:A:2547:C:O2'	58:C:152:LYS:NZ	2.37	0.52
54:A:2167:A:N6	54:A:2212:C:OP2	2.36	0.52
1:D:135:ARG:NH2	54:A:2528:G:OP1	2.43	0.52
26:3:175:ASP:HB3	26:3:178:GLN:HB2	1.91	0.52
47:q:91:GLU:OE1	47:q:92:TRP:NE1	2.43	0.52
17:U:143:ARG:HG3	35:d:282:ILE:HD11	1.91	0.52
54:A:1678:C:N4	54:A:1773:A:OP2	2.35	0.52
59:G:175:LEU:HD21	59:G:178:LYS:HA	1.91	0.52
2:E:135:LYS:NZ	2:E:183:ASP:OD2	2.43	0.52
3:F:142:ARG:NH2	54:A:1794:A:OP1	2.42	0.52
10:N:218:ILE:HA	10:N:223:MET:HG3	1.91	0.52
16:T:97:MET:HE1	16:T:105:GLN:HG3	1.91	0.52
10:N:148:ASP:OD2	10:N:149:HIS:ND1	2.37	0.52
18:V:185:ARG:NH2	18:V:187:TYR:O	2.43	0.52
29:7:114:ASP:OD1	29:7:114:ASP:N	2.42	0.52
17:U:75:GLY:O	17:U:88:LYS:NZ	2.43	0.52
49:s:66:TRP:O	49:s:69:THR:OG1	2.28	0.52
54:A:1962:A:OP2	54:A:2501:C:N4	2.42	0.52
35:d:158:ASP:OD2	35:d:158:ASP:N	2.40	0.51
51:u:138:MET:HG3	51:u:179:LEU:HD22	1.91	0.51
4:H:103:GLU:OE2	4:H:104:ASN:ND2	2.43	0.51
46:p:96:ASN:N	46:p:96:ASN:OD1	2.44	0.51
51:u:172:PHE:HD2	51:u:175:MET:HG3	1.75	0.51
2:E:133:THR:HG1	2:E:144:THR:HG1	1.55	0.51
24:1:22:SER:OG	24:1:23:GLU:N	2.43	0.51
54:A:2182:G:O2'	54:A:2199:A:OP2	2.29	0.51
12:P:54:ARG:NH1	12:P:140:GLY:O	2.44	0.51
18:V:199:MET:HG2	18:V:204:ILE:HD12	1.92	0.51
27:5:276:ASP:OD2	49:s:158:ARG:NH2	2.40	0.51
38:g:143:VAL:HG23	38:g:144:THR:HG23	1.92	0.51
5:I:113:ARG:NH2	54:A:2193:U:O2'	2.43	0.51
12:P:66:ARG:HB2	19:W:92:LEU:HD13	1.91	0.51
22:Z:137:THR:HG22	22:Z:147:VAL:HA	1.92	0.51
27:5:210:SER:HB3	27:5:276:ASP:HB3	1.92	0.51
34:c:179:THR:HG22	34:c:194:THR:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:s:79:LYS:NZ	49:s:344:GLY:O	2.42	0.51
13:Q:118:ARG:HD2	13:Q:175:GLN:HE21	1.76	0.51
17:U:42:PHE:HB2	17:U:95:ALA:HB3	1.93	0.51
19:W:77:PRO:HG3	19:W:83:VAL:HG22	1.92	0.51
20:X:77:ARG:NH1	27:5:46:LEU:O	2.39	0.51
23:0:106:ASN:HB2	23:0:118:GLN:HG3	1.93	0.51
28:6:259:PRO:HG3	28:6:321:CYS:HB3	1.93	0.51
33:b:28:ARG:NE	33:b:78:GLU:OE1	2.44	0.51
51:u:166:ASP:OD1	51:u:166:ASP:N	2.43	0.51
27:5:391:VAL:HG22	27:5:399:GLU:HB2	1.93	0.51
36:e:128:PHE:HB2	44:m:73:ARG:HB3	1.93	0.51
54:A:1814:A:N3	54:A:1862:U:O2'	2.44	0.51
55:B:1605:A:H61	55:B:1666:U:H3	1.59	0.51
1:D:125:LYS:HB2	27:5:258:PRO:HD2	1.92	0.51
3:F:214:ASP:OD1	3:F:214:ASP:N	2.44	0.51
36:e:55:ARG:HG3	36:e:149:LEU:HD11	1.93	0.51
59:G:147:VAL:HG11	59:G:182:VAL:HG11	1.93	0.51
6:J:84:GLN:HG3	6:J:85:PRO:HD2	1.93	0.51
15:S:184:ARG:NH2	54:A:2261:C:O2'	2.44	0.51
48:r:149:ARG:HD3	48:r:152:THR:HG21	1.91	0.51
54:A:3060:C:C4	58:C:77:LYS:HB2	2.46	0.51
11:O:9:ILE:N	54:A:2458:A:OP1	2.44	0.51
17:U:11:ARG:HH11	18:V:211:LYS:HB3	1.76	0.51
18:V:50:SER:OG	18:V:51:ASP:N	2.42	0.51
27:5:201:ARG:NH1	27:5:418:TYR:O	2.43	0.51
54:A:2116:C:O2'	54:A:2837:A:N3	2.38	0.51
2:E:252:TRP:O	2:E:255:THR:OG1	2.27	0.50
5:I:97:ALA:HB3	5:I:154:LEU:HB2	1.94	0.50
7:K:27:PRO:HG2	7:K:30:LYS:HB2	1.93	0.50
7:K:78:SER:HB3	7:K:89:GLN:HG2	1.92	0.50
12:P:64:LYS:HA	12:P:97:GLN:HE22	1.76	0.50
23:0:166:SER:N	23:0:169:ASP:OD1	2.43	0.50
33:b:25:GLN:HA	33:b:80:LEU:HD12	1.93	0.50
44:m:54:VAL:HG21	44:m:68:TYR:HD2	1.75	0.50
59:G:215:LYS:HA	59:G:220:LYS:HG2	1.93	0.50
1:D:184:LEU:HD21	1:D:242:ALA:HB3	1.93	0.50
1:D:204:ALA:O	1:D:208:ARG:NH1	2.44	0.50
5:I:127:PRO:O	5:I:131:LEU:N	2.40	0.50
9:M:179:TYR:OH	9:M:260:LYS:NZ	2.40	0.50
27:5:173:ARG:NH1	27:5:348:ASP:O	2.40	0.50
27:5:267:GLU:OE2	27:5:269:ASN:ND2	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:s:269:ASP:HB3	49:s:270:LYS:HE2	1.93	0.50
52:v:15:ALA:HA	52:v:18:ARG:HB2	1.93	0.50
17:U:71:ARG:NH2	17:U:73:GLN:OE1	2.45	0.50
36:e:68:GLU:HA	36:e:71:ALA:HB3	1.94	0.50
8:L:94:PRO:HG2	8:L:97:THR:HG21	1.94	0.50
16:T:48:SER:O	16:T:49:ARG:NH2	2.44	0.50
16:T:134:VAL:HG13	16:T:180:GLU:HG3	1.94	0.50
17:U:144:ARG:NH2	35:d:274:GLN:O	2.45	0.50
49:s:181:VAL:HG12	49:s:200:LEU:HD21	1.94	0.50
11:O:75:MET:HE2	13:Q:267:PHE:HA	1.94	0.50
17:U:44:ILE:HD11	17:U:53:LEU:HG	1.93	0.50
22:Z:90:GLY:O	22:Z:98:GLN:NE2	2.45	0.50
35:d:267:PRO:HG2	35:d:270:ALA:HB2	1.93	0.50
55:B:1628:C:H2'	55:B:1629:A:C8	2.46	0.50
6:J:143:SER:O	54:A:2170:G:N2	2.36	0.50
16:T:113:GLY:HA2	16:T:116:ILE:HD12	1.94	0.50
41:j:83:GLU:OE1	45:o:66:ARG:NH2	2.44	0.50
49:s:93:VAL:HA	49:s:273:LEU:HD11	1.93	0.50
62:v:101:PNS:O27	62:v:101:PNS:O33	2.26	0.50
8:L:117:THR:HG22	8:L:118:ARG:HG2	1.94	0.49
23:0:85:ARG:NH1	54:A:2308:A:OP1	2.38	0.49
24:1:16:ILE:HG13	24:1:36:ARG:HG2	1.93	0.49
34:c:140:PHE:HZ	34:c:212:ALA:HB1	1.77	0.49
8:L:119:ILE:HB	8:L:141:ALA:HA	1.94	0.49
13:Q:84:ARG:O	54:A:3157:C:O2'	2.21	0.49
15:S:181:LYS:NZ	54:A:2296:U:O4	2.45	0.49
33:b:81:ASN:OD1	33:b:81:ASN:N	2.42	0.49
58:C:54:SER:OG	58:C:55:LEU:N	2.45	0.49
29:7:213:ASP:OD2	29:7:271:ARG:NH2	2.41	0.49
31:9:128:PHE:HD1	31:9:135:PHE:HB3	1.78	0.49
45:o:24:PRO:HG2	48:r:169:TRP:HB2	1.94	0.49
49:s:324:PHE:HA	49:s:361:ILE:HD11	1.93	0.49
7:K:52:ASP:O	16:T:206:ARG:NH1	2.45	0.49
24:1:24:ALA:H	24:1:54:VAL:HG11	1.77	0.49
26:3:117:LEU:HD12	26:3:121:LEU:HB2	1.93	0.49
40:i:74:ILE:HD11	40:i:81:ARG:HA	1.94	0.49
51:u:105:ASN:O	51:u:107:ARG:NH1	2.44	0.49
8:L:32:ILE:HD11	8:L:103:ASN:HB3	1.94	0.49
25:2:89:SER:O	25:2:89:SER:OG	2.28	0.49
44:m:41:THR:OG1	44:m:42:ARG:N	2.45	0.49
58:C:55:LEU:HD13	58:C:112:LEU:HD22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:97:VAL:HG22	2:E:181:ILE:HD11	1.94	0.49
16:T:85:ASP:OD1	16:T:85:ASP:N	2.39	0.49
16:T:112:LYS:HB2	54:A:2673:G:H5''	1.95	0.49
51:u:159:ILE:HB	51:u:162:LYS:HE3	1.94	0.49
52:v:13:TYR:OH	53:w:117:GLU:OE1	2.31	0.49
2:E:106:MET:HE3	2:E:120:THR:HG23	1.95	0.49
14:R:57:ARG:O	14:R:61:LYS:NZ	2.38	0.49
16:T:50:LYS:HA	16:T:53:LYS:HD2	1.95	0.49
54:A:2695:G:N2	54:A:3059:A:OP2	2.44	0.49
5:I:164:MET:HE3	5:I:168:LEU:HB2	1.95	0.49
24:l:33:LYS:HD2	24:l:65:LEU:HD21	1.95	0.49
27:5:121:LEU:HD21	27:5:128:LEU:HD13	1.95	0.49
48:r:90:SER:HA	48:r:93:ILE:HD12	1.95	0.49
54:A:1782:G:O2'	54:A:1793:G:O6	2.26	0.49
16:T:74:TYR:CZ	16:T:177:LYS:HD3	2.48	0.49
3:F:69:LEU:O	3:F:202:TYR:OH	2.30	0.49
5:I:177:LEU:HG	42:k:22:PRO:HG3	1.94	0.49
28:6:206:TYR:O	28:6:243:ASN:ND2	2.46	0.49
30:8:119:LYS:HG3	55:B:1642:G:H4'	1.95	0.49
34:c:72:ILE:HG12	34:c:178:LEU:HD13	1.95	0.49
35:d:263:THR:OG1	35:d:264:LYS:N	2.38	0.49
52:v:54:GLN:HA	52:v:57:LYS:HB3	1.93	0.49
59:G:185:GLY:N	59:G:208:LEU:O	2.44	0.49
59:G:204:MET:HB3	59:G:229:LYS:HA	1.94	0.49
9:M:56:GLU:HG3	54:A:2015:G:H5'	1.95	0.48
10:N:89:ILE:HD11	10:N:176:LEU:HD22	1.94	0.48
40:i:32:ILE:HD13	54:A:1813:C:H2'	1.95	0.48
3:F:237:LEU:O	47:q:25:TYR:N	2.46	0.48
9:M:177:ALA:HB1	9:M:203:ARG:HH12	1.77	0.48
18:V:61:THR:O	18:V:61:THR:OG1	2.29	0.48
18:V:105:ARG:NH1	18:V:106:GLY:O	2.47	0.48
29:7:45:ASN:HD21	29:7:259:ASP:HA	1.79	0.48
1:D:207:ILE:HG23	1:D:229:PRO:HG3	1.94	0.48
7:K:144:GLU:OE1	33:b:146:ARG:NH2	2.47	0.48
49:s:316:CYS:HB2	49:s:319:GLN:HG3	1.94	0.48
54:A:1822:U:O2	54:A:2707:A:O2'	2.29	0.48
1:D:251:ASP:HB3	1:D:254:LYS:HB2	1.95	0.48
9:M:277:MET:SD	38:g:45:TYR:OH	2.68	0.48
9:M:295:THR:HG22	46:p:39:PHE:HE1	1.79	0.48
49:s:87:GLN:O	49:s:277:GLN:NE2	2.46	0.48
5:I:86:ILE:HG21	5:I:131:LEU:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:5:211:ALA:HB1	27:5:322:LEU:HD23	1.94	0.48
33:b:65:VAL:HB	39:h:154:ILE:HG12	1.96	0.48
36:e:67:GLN:O	36:e:71:ALA:N	2.45	0.48
54:A:2459:A:N6	54:A:2668:A:O2'	2.47	0.48
5:I:100:GLN:OE1	42:k:31:ARG:NE	2.45	0.48
21:Y:229:LYS:NZ	54:A:1770:G:O6	2.45	0.48
23:0:114:GLY:HA3	29:7:73:THR:HB	1.96	0.48
27:5:112:ARG:NH2	27:5:303:ARG:O	2.41	0.48
34:c:221:THR:O	34:c:224:THR:OG1	2.28	0.48
38:g:96:VAL:HG22	38:g:110:ILE:HG12	1.96	0.48
49:s:307:ARG:NH2	54:A:2416:U:O4	2.46	0.48
5:I:161:VAL:HA	5:I:164:MET:HB3	1.94	0.48
54:A:1935:A:O2'	54:A:1938:A:N6	2.46	0.48
1:D:206:TYR:O	1:D:208:ARG:N	2.34	0.48
9:M:192:PRO:HB3	54:A:1887:A:H2	1.78	0.48
28:6:380:TYR:OH	54:A:1892:A:OP2	2.26	0.48
36:e:142:GLU:HB3	36:e:145:ASP:HB2	1.95	0.48
42:k:29:SER:HB2	42:k:86:MET:HE1	1.96	0.48
54:A:2180:A:O2'	54:A:2206:C:O3'	2.32	0.48
58:C:105:ARG:HE	58:C:106:LYS:HD3	1.79	0.48
3:F:110:SER:HB3	3:F:161:TYR:HE1	1.79	0.48
7:K:10:GLN:NE2	16:T:206:ARG:O	2.35	0.48
13:Q:123:ASP:OD1	13:Q:131:SER:OG	2.32	0.48
18:V:147:SER:OG	18:V:150:SER:O	2.26	0.48
21:Y:198:ARG:HD3	54:A:1712:A:H2	1.78	0.48
31:9:28:ARG:HD3	54:A:2337:A:H5''	1.96	0.48
39:h:148:LEU:HD22	39:h:152:LEU:HD13	1.96	0.48
52:v:16:LEU:HD13	52:v:35:ILE:HD12	1.95	0.48
56:24:51:G:H21	56:24:52:C:H5	1.60	0.48
1:D:221:ASN:OD1	1:D:221:ASN:N	2.47	0.47
9:M:149:THR:O	9:M:149:THR:OG1	2.27	0.47
17:U:19:VAL:HG22	31:9:136:LEU:HD23	1.95	0.47
36:e:192:LEU:HD21	36:e:200:MET:HB2	1.96	0.47
42:k:82:THR:HG22	42:k:84:LEU:H	1.79	0.47
52:v:46:GLU:H	52:v:51:ARG:HH21	1.61	0.47
52:v:47:ASP:OD2	52:v:47:ASP:N	2.44	0.47
55:B:1628:C:H2'	55:B:1629:A:H8	1.79	0.47
5:I:83:ARG:HA	5:I:134:PHE:CE2	2.48	0.47
8:L:87:VAL:HG12	8:L:127:LEU:HD11	1.96	0.47
11:O:50:ASP:HA	11:O:53:ARG:HB2	1.96	0.47
22:Z:101:LYS:HB2	22:Z:103:ILE:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:7:241:GLU:O	29:7:245:SER:OG	2.28	0.47
49:s:228:ASP:OD2	49:s:230:ARG:NH1	2.47	0.47
17:U:46:MET:HE1	17:U:72:VAL:HG13	1.95	0.47
30:8:113:ARG:HA	30:8:116:LEU:HB2	1.95	0.47
41:j:77:VAL:O	41:j:81:SER:OG	2.25	0.47
49:s:321:GLU:OE2	49:s:397:GLN:NE2	2.47	0.47
12:P:157:SER:OG	55:B:1640:A:OP1	2.26	0.47
29:7:60:PRO:HG2	29:7:63:GLU:HB2	1.97	0.47
29:7:243:LYS:HA	29:7:243:LYS:HD3	1.68	0.47
58:C:151:LYS:HA	58:C:154:LEU:HG	1.97	0.47
6:J:108:VAL:HG21	6:J:154:ARG:HH21	1.80	0.47
7:K:73:GLU:OE2	48:r:149:ARG:NH2	2.46	0.47
9:M:243:ILE:HG12	46:p:73:LEU:HD12	1.96	0.47
11:O:70:GLU:OE1	11:O:74:ARG:NH1	2.47	0.47
28:6:232:TYR:HE1	28:6:297:THR:HG22	1.79	0.47
33:b:4:ARG:NH2	54:A:1837:C:OP1	2.48	0.47
36:e:152:LYS:HE3	36:e:155:ARG:HD2	1.97	0.47
36:e:248:ASN:HB2	36:e:252:HIS:HE1	1.80	0.47
46:p:111:ILE:O	46:p:116:ARG:NH1	2.48	0.47
49:s:232:GLN:HE22	49:s:281:HIS:H	1.62	0.47
58:C:128:HIS:HD2	58:C:131:LYS:HD3	1.79	0.47
1:D:259:LYS:HG2	1:D:262:ARG:HG3	1.96	0.47
2:E:275:ARG:NH2	2:E:331:ASP:OD2	2.48	0.47
16:T:47:ILE:N	54:A:1674:A:N7	2.63	0.47
20:X:23:ARG:NH2	20:X:219:GLU:OE1	2.47	0.47
59:G:163:PHE:HB2	59:G:168:LEU:HD12	1.96	0.47
26:3:148:VAL:HG13	28:6:360:ARG:HA	1.97	0.47
42:k:86:MET:HE3	42:k:86:MET:HB2	1.71	0.47
54:A:3008:C:O2'	54:A:3051:A:N3	2.47	0.47
8:L:37:ARG:HH12	8:L:56:ARG:HH11	1.63	0.47
20:X:56:ASN:OD1	20:X:56:ASN:N	2.48	0.47
36:e:184:LEU:HB3	36:e:234:PHE:HZ	1.80	0.47
46:p:124:LYS:HA	46:p:127:ILE:HD12	1.96	0.47
49:s:405:ILE:HG12	49:s:410:VAL:HB	1.96	0.47
2:E:202:GLN:NE2	2:E:301:ASP:OD1	2.48	0.46
8:L:33:GLN:HG2	8:L:66:VAL:HG12	1.96	0.46
29:7:121:LYS:HB3	29:7:121:LYS:HE2	1.77	0.46
10:N:61:LYS:HD2	10:N:130:PRO:HD3	1.97	0.46
10:N:108:THR:HG22	10:N:111:ARG:HH21	1.79	0.46
16:T:149:ARG:NH2	54:A:1673:U:O2'	2.48	0.46
11:O:32:LEU:HB3	11:O:52:MET:HE2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:S:87:ILE:HG22	15:S:202:PRO:HG3	1.98	0.46
16:T:132:HIS:CD2	35:d:227:ARG:HE	2.33	0.46
34:c:210:ARG:HD2	34:c:210:ARG:HA	1.71	0.46
48:r:86:VAL:HA	48:r:89:LEU:HB2	1.98	0.46
49:s:76:VAL:HA	49:s:79:LYS:HB2	1.97	0.46
54:A:2017:U:O2'	54:A:2723:A:N1	2.46	0.46
14:R:11:ARG:HB2	54:A:2292:G:H2'	1.97	0.46
30:8:112:GLU:O	30:8:116:LEU:N	2.48	0.46
41:j:24:GLY:O	41:j:28:ARG:NH2	2.49	0.46
6:J:47:ASN:O	6:J:51:LYS:N	2.46	0.46
8:L:69:VAL:HG22	8:L:88:GLY:H	1.80	0.46
27:5:333:ALA:HB1	27:5:363:ASP:HA	1.98	0.46
44:m:69:ARG:HD2	44:m:70:GLU:HG2	1.96	0.46
48:r:154:TRP:HB3	54:A:3189:C:H1'	1.97	0.46
2:E:154:ARG:HH22	29:7:315:LYS:HZ1	1.62	0.46
7:K:32:ALA:HB3	7:K:111:MET:HE3	1.97	0.46
26:3:111:ILE:HD13	26:3:111:ILE:HA	1.80	0.46
34:c:122:ASN:HD21	34:c:194:THR:HA	1.80	0.46
48:r:182:ARG:HH22	54:A:2157:U:H5'	1.81	0.46
56:24:9:A:H8	56:24:11:C:H41	1.64	0.46
6:J:69:LYS:HE3	6:J:129:ALA:HB1	1.98	0.46
17:U:66:ALA:HB2	17:U:100:ALA:HB2	1.98	0.46
18:V:100:LYS:HD3	57:Y2:3:UNK:H	1.81	0.46
28:6:224:HIS:CE1	28:6:227:GLU:H	2.33	0.46
31:9:53:ILE:HD12	31:9:56:MET:HE3	1.96	0.46
35:d:208:VAL:HG22	35:d:252:LEU:HD12	1.97	0.46
46:p:125:ASN:N	46:p:125:ASN:OD1	2.47	0.46
49:s:247:LEU:HD11	49:s:296:HIS:HA	1.98	0.46
22:Z:84:ASP:HB3	22:Z:88:MET:HE3	1.98	0.46
23:0:163:GLU:OE1	23:0:181:ARG:NH2	2.49	0.46
28:6:169:PRO:HB3	28:6:316:LEU:HB2	1.98	0.46
37:f:122:GLU:HB2	37:f:158:GLN:HB3	1.98	0.46
39:h:101:LEU:HD22	39:h:112:VAL:HG21	1.98	0.46
45:o:23:ARG:NH1	54:A:2131:A:OP1	2.42	0.46
47:q:61:PHE:HB2	47:q:70:VAL:HG22	1.97	0.46
49:s:67:GLN:O	49:s:71:HIS:ND1	2.48	0.46
7:K:39:LEU:HD11	7:K:125:LEU:HD13	1.97	0.46
9:M:62:ARG:NH1	40:i:126:LYS:O	2.42	0.45
15:S:122:LEU:HD13	15:S:128:ILE:HD11	1.98	0.45
17:U:82:HIS:H	17:U:82:HIS:CD2	2.34	0.45
28:6:29:THR:OG1	37:f:50:THR:O	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:c:166:VAL:HG11	34:c:192:GLN:HG3	1.97	0.45
53:w:143:GLU:O	53:w:147:TYR:N	2.49	0.45
8:L:73:ILE:HD11	8:L:105:VAL:HG21	1.97	0.45
9:M:17:ARG:HH22	39:h:119:GLN:HE21	1.65	0.45
23:0:179:ARG:HH11	23:0:182:PRO:HG3	1.81	0.45
38:g:150:LYS:NZ	54:A:2052:A:OP1	2.48	0.45
11:O:131:PRO:HB2	23:0:130:VAL:HG13	1.99	0.45
47:q:48:PRO:HG2	47:q:51:GLN:HG3	1.99	0.45
26:3:159:ASP:O	26:3:167:LYS:NZ	2.36	0.45
31:9:22:THR:HG23	31:9:24:LYS:H	1.82	0.45
49:s:271:LEU:O	49:s:273:LEU:N	2.50	0.45
54:A:1679:U:O2'	54:A:1680:A:OP2	2.34	0.45
1:D:194:ASN:OD1	1:D:243:THR:OG1	2.34	0.45
9:M:56:GLU:OE1	54:A:2040:G:O2'	2.30	0.45
20:X:167:LEU:HD11	20:X:202:GLU:HG2	1.98	0.45
23:0:119:LYS:O	23:0:120:HIS:ND1	2.49	0.45
5:I:148:VAL:HG21	42:k:28:GLU:HG3	1.97	0.45
6:J:132:LEU:HD22	6:J:140:VAL:HG22	1.98	0.45
12:P:130:ARG:HD3	28:6:132:LEU:HD21	1.99	0.45
14:R:104:ASP:OD2	16:T:211:THR:OG1	2.35	0.45
21:Y:93:LYS:HE2	31:9:70:LEU:HD11	1.99	0.45
22:Z:36:PHE:CE2	22:Z:79:PRO:HG3	2.51	0.45
24:1:61:LYS:HE2	24:1:61:LYS:HB2	1.76	0.45
49:s:90:LYS:HD2	49:s:232:GLN:HB2	1.98	0.45
7:K:34:MET:HE2	7:K:34:MET:HB3	1.76	0.45
21:Y:111:MET:HE3	21:Y:111:MET:HB3	1.86	0.45
29:7:99:TYR:O	29:7:103:SER:OG	2.24	0.45
35:d:230:ARG:H	35:d:230:ARG:HG2	1.58	0.45
58:C:50:PRO:HB2	58:C:126:PRO:HB3	1.98	0.45
4:H:119:GLY:HA2	4:H:123:LEU:HB2	1.98	0.45
27:5:173:ARG:NH2	54:A:2395:A:OP1	2.38	0.45
48:r:41:THR:O	48:r:41:THR:OG1	2.27	0.45
53:w:87:LEU:HD13	53:w:98:LEU:HD11	1.97	0.45
17:U:79:ARG:HE	17:U:79:ARG:HB2	1.66	0.45
27:5:123:LEU:HD12	27:5:315:LEU:HD11	1.98	0.45
40:i:126:LYS:HE2	54:A:2093:U:H4'	1.97	0.45
49:s:113:VAL:HG23	49:s:392:ILE:HG23	1.98	0.45
54:A:1747:G:OP2	54:A:1749:C:N4	2.50	0.45
54:A:1835:A:O2'	54:A:1836:A:N7	2.44	0.45
5:I:126:PHE:HB2	5:I:131:LEU:HD22	1.99	0.45
21:Y:122:GLN:HB3	21:Y:124:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:w:79:ILE:HA	53:w:126:PHE:HE2	1.82	0.45
58:C:140:GLU:OE2	58:C:143:LYS:NZ	2.34	0.45
8:L:68:LYS:N	8:L:71:ASP:OD2	2.44	0.44
28:6:102:GLN:O	28:6:106:ARG:N	2.39	0.44
45:o:15:ARG:NH2	54:A:2134:A:OP1	2.50	0.44
46:p:42:ILE:HA	46:p:47:LYS:HD2	1.99	0.44
54:A:2029:A:O2'	54:A:2124:A:N6	2.50	0.44
5:I:34:THR:OG1	5:I:36:HIS:O	2.32	0.44
17:U:83:ARG:HB2	17:U:85:VAL:HG23	2.00	0.44
27:5:198:LEU:HD11	27:5:419:LEU:HD23	1.99	0.44
37:f:117:LEU:HD13	37:f:166:PHE:HZ	1.82	0.44
8:L:133:GLU:HG3	51:u:160:GLU:HB3	1.99	0.44
13:Q:154:VAL:HA	13:Q:159:GLY:HA2	2.00	0.44
22:Z:35:LYS:HB3	54:A:2119:U:H1'	1.98	0.44
27:5:147:ILE:HD11	27:5:411:PHE:HE2	1.81	0.44
51:u:138:MET:H	51:u:138:MET:HG2	1.62	0.44
59:G:131:ASN:HB3	59:G:228:TRP:CD1	2.52	0.44
21:Y:216:ARG:HE	21:Y:216:ARG:HB2	1.47	0.44
22:Z:148:GLN:OE1	22:Z:150:HIS:NE2	2.50	0.44
27:5:339:PRO:HB3	27:5:360:ASN:HB3	1.99	0.44
28:6:166:THR:OG1	28:6:167:PHE:N	2.49	0.44
48:r:182:ARG:NH1	54:A:2157:U:OP1	2.50	0.44
49:s:332:LEU:HD23	49:s:332:LEU:HA	1.84	0.44
51:u:181:LEU:HD23	51:u:181:LEU:HA	1.84	0.44
54:A:1955:G:O2'	54:A:1958:G:O2'	2.32	0.44
59:G:150:THR:O	59:G:150:THR:OG1	2.34	0.44
13:Q:97:LYS:HE2	13:Q:97:LYS:HB3	1.90	0.44
18:V:133:ILE:HD13	18:V:133:ILE:HA	1.83	0.44
19:W:104:TYR:HB2	19:W:128:LYS:HG2	2.00	0.44
20:X:136:ASP:OD1	20:X:136:ASP:N	2.46	0.44
32:a:62:HIS:O	32:a:62:HIS:ND1	2.48	0.44
37:f:60:LYS:HE3	37:f:60:LYS:HB3	1.91	0.44
14:R:35:LYS:HE2	14:R:35:LYS:HB2	1.69	0.44
22:Z:36:PHE:HE2	22:Z:79:PRO:HG3	1.83	0.44
27:5:232:THR:OG1	27:5:234:ASP:O	2.31	0.44
28:6:72:ARG:HG3	54:A:2063:G:H5'	2.00	0.44
54:A:2181:A:N7	54:A:2206:C:O2'	2.43	0.44
5:I:51:THR:O	5:I:51:THR:OG1	2.34	0.44
9:M:28:LYS:HE3	9:M:28:LYS:HB3	1.87	0.44
9:M:107:LEU:HD23	9:M:107:LEU:HA	1.82	0.44
19:W:62:HIS:HA	19:W:94:GLU:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:7:41:THR:OG1	29:7:259:ASP:O	2.36	0.44
36:e:97:ARG:HA	36:e:100:LYS:HB2	2.00	0.44
36:e:264:LEU:HD22	36:e:269:LEU:HB3	1.99	0.44
54:A:2959:G:H2'	54:A:2962:C:H42	1.83	0.44
13:Q:240:ILE:HG22	13:Q:242:GLY:H	1.82	0.44
17:U:147:VAL:HG22	35:d:232:MET:HE2	2.00	0.44
21:Y:140:ASP:N	21:Y:140:ASP:OD1	2.50	0.44
33:b:44:ARG:NH2	45:o:99:LYS:O	2.51	0.44
34:c:72:ILE:HD12	34:c:89:LYS:HG2	2.00	0.44
40:i:102:MET:HE1	40:i:110:LEU:HD22	1.99	0.44
59:G:188:LEU:HB2	59:G:206:ILE:HB	1.99	0.44
12:P:122:VAL:HG22	12:P:157:SER:HB3	1.99	0.44
17:U:123:ALA:H	17:U:127:TYR:HB2	1.83	0.44
27:5:61:ALA:HB2	27:5:73:PRO:HG3	2.00	0.44
28:6:359:HIS:CE1	28:6:360:ARG:HG3	2.52	0.44
30:8:114:ARG:HG3	36:e:73:LEU:HD11	1.99	0.44
36:e:146:ARG:HG2	36:e:253:VAL:HG23	1.98	0.44
41:j:97:LYS:HA	41:j:97:LYS:HD2	1.77	0.44
44:m:54:VAL:HB	44:m:68:TYR:HB3	2.00	0.44
51:u:119:ARG:H	51:u:119:ARG:HG2	1.44	0.44
54:A:2586:U:H5'	59:G:155:GLY:HA3	2.00	0.44
3:F:278:SER:O	3:F:278:SER:OG	2.31	0.43
13:Q:182:ARG:HG3	13:Q:187:LEU:HD11	2.00	0.43
26:3:101:LYS:HB2	26:3:103:LYS:HG3	2.00	0.43
47:q:150:LYS:HA	47:q:150:LYS:HD2	1.83	0.43
48:r:94:ARG:NH2	54:A:3181:U:OP1	2.50	0.43
52:v:27:ASP:O	52:v:31:TYR:N	2.44	0.43
59:G:171:ASN:ND2	59:G:186:ASP:O	2.51	0.43
10:N:224:LEU:HD23	45:o:35:MET:HE3	1.99	0.43
54:A:1953:A:O2'	54:A:2463:A:OP1	2.33	0.43
54:A:2187:C:H2'	54:A:2188:A:H8	1.83	0.43
54:A:2795:U:H2'	54:A:2796:G:C8	2.53	0.43
2:E:266:ARG:HA	2:E:266:ARG:HD3	1.67	0.43
5:I:123:MET:HB3	5:I:154:LEU:HD23	2.01	0.43
9:M:14:ASP:OD1	9:M:14:ASP:N	2.48	0.43
24:1:20:MET:HA	24:1:58:GLU:HA	2.00	0.43
27:5:124:THR:O	27:5:372:ASN:ND2	2.51	0.43
38:g:118:TRP:NE1	38:g:142:GLU:OE2	2.37	0.43
49:s:60:LEU:HD23	49:s:63:ILE:HD12	2.01	0.43
49:s:228:ASP:OD2	49:s:228:ASP:N	2.49	0.43
53:w:80:GLN:HG2	53:w:145:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:A:2273:A:N1	54:A:2293:A:O2'	2.50	0.43
8:L:47:GLY:HA2	8:L:77:ILE:HD11	2.01	0.43
33:b:111:ASP:HB3	33:b:113:ILE:HG23	2.01	0.43
33:b:140:PHE:CZ	33:b:141:ARG:HD3	2.53	0.43
48:r:87:LEU:HD23	48:r:87:LEU:HA	1.88	0.43
54:A:2928:C:OP2	54:A:3073:C:O2'	2.35	0.43
2:E:154:ARG:HB3	29:7:311:THR:HG21	1.99	0.43
7:K:135:GLU:HA	7:K:138:LEU:HB2	2.01	0.43
12:P:87:GLN:HE22	55:B:1625:A:H62	1.66	0.43
20:X:86:ILE:HB	20:X:105:TRP:HB2	2.01	0.43
22:Z:105:SER:OG	45:o:59:GLU:OE2	2.31	0.43
36:e:44:PRO:O	36:e:228:GLY:N	2.43	0.43
12:P:85:ARG:HD2	12:P:158:MET:HE3	2.01	0.43
13:Q:165:GLU:HB2	13:Q:168:ASN:HB2	2.00	0.43
39:h:120:MET:HB3	39:h:120:MET:HE2	1.70	0.43
49:s:105:TRP:CG	49:s:271:LEU:HD13	2.54	0.43
54:A:2695:G:OP1	54:A:2941:G:O2'	2.35	0.43
54:A:2987:U:O2'	54:A:2991:U:OP1	2.32	0.43
10:N:221:ALA:O	22:Z:114:LYS:NZ	2.50	0.43
13:Q:240:ILE:HG21	13:Q:243:ILE:HG12	1.99	0.43
34:c:140:PHE:HB3	34:c:314:TRP:HZ2	1.83	0.43
36:e:79:ILE:HG22	44:m:50:ARG:HH21	1.84	0.43
46:p:38:GLU:HB3	46:p:39:PHE:H	1.69	0.43
47:q:109:ALA:O	47:q:113:LYS:N	2.49	0.43
54:A:2194:U:O2'	54:A:2195:A:O5'	2.35	0.43
2:E:100:ILE:HD11	2:E:177:LYS:HB2	2.00	0.43
3:F:49:ARG:NH1	3:F:270:GLU:OE1	2.48	0.43
6:J:39:LEU:O	6:J:43:GLY:N	2.50	0.43
9:M:93:TYR:HE2	26:3:173:VAL:HG22	1.84	0.43
9:M:175:THR:HG21	9:M:259:ARG:HD3	2.00	0.43
11:O:18:MET:HE3	11:O:48:ARG:HG2	2.01	0.43
27:5:343:GLN:HB3	27:5:356:VAL:HG13	2.00	0.43
30:8:130:LYS:HE3	30:8:130:LYS:HB3	1.89	0.43
36:e:117:ALA:HA	36:e:120:LEU:HD12	2.01	0.43
42:k:19:GLN:HG3	42:k:56:ARG:HE	1.83	0.43
3:F:82:LEU:HD22	3:F:266:VAL:HG11	2.00	0.43
3:F:160:SER:HB2	40:i:80:LEU:HD13	2.01	0.43
12:P:160:ARG:HD3	12:P:160:ARG:HA	1.85	0.43
15:S:86:MET:HE2	15:S:86:MET:HB3	1.89	0.43
20:X:79:LEU:HD23	20:X:79:LEU:HA	1.86	0.43
28:6:265:ILE:HG13	28:6:322:ARG:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:6:297:THR:O	28:6:297:THR:OG1	2.27	0.43
31:9:31:ARG:HD2	54:A:2421:G:H4'	2.01	0.43
33:b:77:ALA:HB2	33:b:104:LEU:HD13	2.00	0.43
1:D:232:ARG:NH1	1:D:291:PRO:O	2.52	0.43
5:I:49:ALA:HB1	45:o:32:LYS:HE2	2.00	0.43
20:X:117:GLU:N	20:X:142:ASP:OD2	2.52	0.43
27:5:208:THR:HG22	27:5:225:SER:HB3	2.00	0.43
35:d:165:THR:HG23	35:d:167:HIS:H	1.84	0.43
48:r:132:ARG:HA	48:r:132:ARG:HD2	1.70	0.43
2:E:257:MET:SD	54:A:2712:G:N2	2.92	0.42
3:F:63:GLN:HA	3:F:81:ASP:HA	2.00	0.42
4:H:99:THR:OG1	4:H:128:LEU:O	2.24	0.42
6:J:124:LYS:HD2	6:J:124:LYS:HA	1.84	0.42
8:L:100:PHE:HE2	8:L:122:PRO:HG2	1.84	0.42
10:N:67:LYS:HE2	54:A:2110:A:H5'	2.01	0.42
13:Q:177:VAL:HG13	13:Q:206:PRO:HA	2.01	0.42
14:R:12:ASN:OD1	14:R:12:ASN:N	2.50	0.42
18:V:96:ARG:HE	18:V:111:SER:HB3	1.84	0.42
22:Z:125:PRO:HD3	22:Z:144:GLU:HB2	2.00	0.42
24:1:55:LEU:HD21	47:q:135:TRP:CG	2.54	0.42
28:6:233:LEU:HB3	28:6:298:PHE:CD1	2.54	0.42
35:d:88:TYR:CZ	35:d:195:VAL:HG11	2.54	0.42
49:s:243:ILE:HD11	49:s:247:LEU:HG	2.01	0.42
52:v:65:LYS:HB3	52:v:66:LEU:HD12	2.01	0.42
55:B:1648:U:H2'	55:B:1649:C:H6	1.84	0.42
16:T:111:LYS:HE3	23:0:101:ILE:HD11	2.01	0.42
18:V:107:THR:HG22	57:Y2:1:UNK:H2	1.83	0.42
20:X:209:GLU:HA	20:X:212:ILE:HD12	2.01	0.42
36:e:162:ARG:HB2	36:e:171:TRP:CE2	2.54	0.42
49:s:85:LYS:HE2	54:A:2446:A:N6	2.34	0.42
53:w:110:LEU:HD23	53:w:110:LEU:HA	1.90	0.42
56:24:4:A:H2'	56:24:5:A:C8	2.54	0.42
10:N:163:MET:HE3	10:N:163:MET:HB3	1.68	0.42
12:P:44:VAL:HG13	28:6:225:LEU:HB3	2.01	0.42
27:5:336:LEU:HD23	27:5:336:LEU:HA	1.90	0.42
33:b:37:GLY:H	33:b:44:ARG:HH12	1.67	0.42
51:u:177:ILE:HG22	51:u:179:LEU:HG	2.00	0.42
3:F:50:LYS:HD3	3:F:50:LYS:HA	1.65	0.42
27:5:132:LEU:HD22	27:5:356:VAL:HG23	2.02	0.42
34:c:47:ARG:HE	34:c:47:ARG:HB3	1.68	0.42
49:s:192:ASN:HB3	49:s:195:LEU:HD22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:w:93:ILE:HD13	53:w:93:ILE:HA	1.88	0.42
54:A:3051:A:OP1	54:A:3116:C:O2'	2.38	0.42
3:F:195:LEU:HD22	3:F:202:TYR:HE2	1.84	0.42
7:K:118:ARG:HA	7:K:121:MET:HE3	2.02	0.42
10:N:140:MET:HB3	10:N:140:MET:HE3	1.74	0.42
13:Q:100:LEU:HD11	13:Q:286:ILE:HD13	2.01	0.42
32:a:69:TYR:CG	34:c:278:LYS:HG3	2.54	0.42
51:u:111:VAL:H	52:v:26:THR:HG22	1.83	0.42
55:B:1661:A:N6	55:B:1663:C:N3	2.67	0.42
5:I:77:GLY:HA2	5:I:80:ARG:HG2	2.02	0.42
9:M:72:THR:HA	9:M:73:PRO:HD3	1.93	0.42
10:N:86:ASN:HA	10:N:192:ARG:HG3	2.00	0.42
12:P:118:SER:HG	12:P:121:ASN:ND2	2.16	0.42
12:P:144:MET:SD	12:P:144:MET:N	2.92	0.42
13:Q:289:SER:O	13:Q:289:SER:OG	2.29	0.42
14:R:112:THR:HG23	15:S:142:THR:HG21	2.01	0.42
16:T:94:ILE:HA	16:T:97:MET:HG3	2.00	0.42
17:U:110:LEU:HD12	21:Y:118:GLU:HG2	2.00	0.42
23:O:155:GLU:HB2	23:O:172:LYS:HD3	2.02	0.42
25:2:51:ASN:O	25:2:54:GLN:NE2	2.53	0.42
26:3:183:ARG:HD2	26:3:183:ARG:HA	1.63	0.42
27:5:351:VAL:HG23	27:5:379:ASP:HA	2.01	0.42
29:7:139:ASN:HB3	29:7:174:VAL:HG21	2.00	0.42
36:e:59:VAL:HG21	36:e:153:LEU:HD23	2.00	0.42
46:p:104:HIS:HA	46:p:132:GLU:HA	2.01	0.42
49:s:191:HIS:O	49:s:428:ARG:NH2	2.52	0.42
12:P:130:ARG:HB3	28:6:132:LEU:HD11	2.01	0.42
17:U:29:VAL:HG12	21:Y:117:GLN:HG2	2.01	0.42
27:5:117:VAL:O	27:5:121:LEU:HG	2.20	0.42
29:7:51:GLU:HG3	29:7:225:VAL:HG11	2.02	0.42
40:i:128:ARG:HE	40:i:128:ARG:HB3	1.41	0.42
43:l:124:GLN:HA	43:l:127:TRP:HB2	2.00	0.42
46:p:75:ARG:HD3	46:p:75:ARG:HA	1.92	0.42
51:u:197:ARG:HD2	51:u:197:ARG:HA	1.68	0.42
52:v:2:ALA:HB1	52:v:48:ALA:HA	2.00	0.42
52:v:46:GLU:O	52:v:51:ARG:NH2	2.53	0.42
1:D:232:ARG:HD2	1:D:290:PRO:HG2	2.01	0.42
5:I:79:ILE:O	5:I:83:ARG:N	2.52	0.42
19:W:100:THR:OG1	19:W:132:HIS:NE2	2.38	0.42
24:1:50:VAL:HG23	24:1:52:GLN:HB2	2.02	0.42
28:6:260:ALA:O	28:6:263:SER:OG	2.30	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:C:86:HIS:CE1	58:C:116:VAL:HG21	2.55	0.42
3:F:196:PRO:HG2	3:F:197:THR:HG22	2.02	0.42
6:J:26:ALA:HB1	6:J:57:THR:HG23	2.01	0.42
11:O:109:GLN:HG2	23:O:121:VAL:HG22	2.02	0.42
11:O:116:ASP:OD2	54:A:2453:G:O2'	2.33	0.42
12:P:96:HIS:HB3	12:P:98:ASN:H	1.85	0.42
35:d:142:LYS:HB3	35:d:142:LYS:HE2	1.80	0.42
3:F:63:GLN:OE1	39:h:97:LYS:NZ	2.38	0.42
13:Q:283:TRP:O	13:Q:287:GLU:HG2	2.20	0.42
24:1:20:MET:HE3	24:1:20:MET:HB3	1.76	0.42
34:c:128:GLN:HG2	34:c:203:LEU:HD22	2.02	0.42
34:c:274:LEU:HD23	34:c:274:LEU:HA	1.88	0.42
39:h:62:PRO:HB3	39:h:131:ASN:HA	2.01	0.42
47:q:55:ARG:HD2	47:q:55:ARG:HA	1.89	0.42
58:C:118:VAL:HG22	58:C:127:VAL:HG21	2.02	0.42
6:J:120:ILE:HG22	6:J:123:ILE:HD11	2.02	0.41
9:M:117:ASP:H	9:M:120:GLN:HB2	1.85	0.41
13:Q:129:LYS:HD2	51:u:119:ARG:HA	2.00	0.41
13:Q:204:MET:HE3	13:Q:204:MET:HB2	1.88	0.41
14:R:141:ILE:HG22	32:a:51:LEU:HD12	2.02	0.41
22:Z:101:LYS:NZ	54:A:2082:G:OP1	2.48	0.41
27:5:126:THR:HG21	27:5:357:PHE:HE1	1.85	0.41
42:k:68:PHE:HB2	42:k:72:HIS:HB2	2.01	0.41
46:p:128:ASN:OD1	46:p:129:ARG:N	2.53	0.41
3:F:113:LYS:HD2	3:F:157:GLY:HA2	2.01	0.41
11:O:42:ILE:HD13	11:O:42:ILE:HA	1.87	0.41
13:Q:86:ARG:H	13:Q:86:ARG:HG2	1.57	0.41
15:S:155:ARG:NE	15:S:157:GLU:OE2	2.52	0.41
20:X:182:GLU:H	20:X:182:GLU:HG3	1.67	0.41
30:8:135:THR:HB	30:8:139:MET:HE3	2.02	0.41
36:e:74:LEU:HD23	36:e:74:LEU:HA	1.92	0.41
38:g:124:VAL:HG21	38:g:147:LEU:HD21	2.02	0.41
38:g:162:LEU:HD23	38:g:162:LEU:HA	1.82	0.41
43:l:133:SER:O	43:l:133:SER:OG	2.32	0.41
54:A:3131:G:H3'	54:A:3132:G:H8	1.86	0.41
1:D:90:ARG:NH2	54:A:1984:A:OP1	2.42	0.41
1:D:269:ARG:HH11	1:D:269:ARG:HD2	1.73	0.41
20:X:97:LEU:HD23	20:X:97:LEU:HA	1.88	0.41
20:X:187:ILE:HA	20:X:187:ILE:HD13	1.83	0.41
29:7:285:ASN:HB3	29:7:293:LEU:HD11	2.03	0.41
34:c:240:LEU:HD12	34:c:240:LEU:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:d:290:GLU:OE1	35:d:290:GLU:N	2.53	0.41
49:s:310:ARG:HE	49:s:310:ARG:HB2	1.54	0.41
53:w:97:LYS:HE2	53:w:97:LYS:HB2	1.82	0.41
54:A:1851:G:H2'	54:A:2693:A:N7	2.35	0.41
2:E:99:LEU:HD13	2:E:124:VAL:HG21	2.02	0.41
2:E:99:LEU:HD23	2:E:99:LEU:HA	1.83	0.41
9:M:41:ARG:NE	54:A:2294:A:OP2	2.41	0.41
11:O:16:ARG:HB3	11:O:18:MET:HG3	2.02	0.41
11:O:41:ARG:NH2	11:O:131:PRO:O	2.38	0.41
14:R:83:TYR:CE1	14:R:87:ILE:HG13	2.55	0.41
15:S:161:ILE:HG23	33:b:17:ASN:HD22	1.85	0.41
18:V:103:ASP:OD2	18:V:103:ASP:N	2.47	0.41
21:Y:189:HIS:CD2	21:Y:190:LEU:HD23	2.56	0.41
26:3:168:ARG:NH2	54:A:1890:C:OP2	2.53	0.41
26:3:188:VAL:HG11	38:g:104:ASN:HB3	2.02	0.41
27:5:142:ASP:OD1	27:5:142:ASP:N	2.39	0.41
38:g:89:SER:OG	38:g:90:ARG:N	2.52	0.41
41:j:88:LEU:HD23	41:j:88:LEU:HA	1.89	0.41
45:o:46:HIS:O	45:o:50:SER:OG	2.32	0.41
46:p:97:SER:OG	46:p:98:LYS:N	2.53	0.41
54:A:2177:U:N3	54:A:2180:A:OP2	2.51	0.41
5:I:33:VAL:HG13	10:N:244:LYS:HB3	2.01	0.41
9:M:279:ASP:OD2	9:M:279:ASP:N	2.49	0.41
13:Q:219:GLU:H	13:Q:219:GLU:HG2	1.42	0.41
15:S:68:ASP:HB3	15:S:71:GLU:HG3	2.02	0.41
29:7:269:ILE:HG23	29:7:274:ILE:HD12	2.01	0.41
51:u:97:MET:HE2	51:u:177:ILE:HG12	2.01	0.41
6:J:114:LEU:O	6:J:118:TYR:N	2.43	0.41
7:K:28:PRO:HD3	7:K:65:ILE:HG23	2.02	0.41
20:X:97:LEU:HD23	54:A:1728:U:H1'	2.03	0.41
27:5:201:ARG:HE	27:5:201:ARG:HB3	1.59	0.41
28:6:235:TRP:HB3	28:6:254:TYR:HA	2.02	0.41
35:d:60:ALA:O	35:d:64:GLY:N	2.51	0.41
38:g:99:ASP:HB3	38:g:107:MET:HG2	2.03	0.41
44:m:58:LYS:H	44:m:58:LYS:HG3	1.65	0.41
54:A:2506:A:H1'	54:A:2601:A:N6	2.36	0.41
54:A:3219:G:H2'	54:A:3220:A:H5''	2.03	0.41
14:R:32:ARG:H	14:R:35:LYS:HZ1	1.67	0.41
18:V:105:ARG:HE	18:V:105:ARG:HB3	1.75	0.41
18:V:199:MET:HE2	18:V:199:MET:HB3	1.91	0.41
27:5:381:LEU:H	27:5:381:LEU:HG	1.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:c:227:GLU:HB3	34:c:230:GLU:HG3	2.02	0.41
35:d:122:ILE:HD11	35:d:197:VAL:HG21	2.03	0.41
35:d:190:GLU:OE1	35:d:215:ARG:NH2	2.39	0.41
36:e:68:GLU:O	36:e:72:SER:N	2.54	0.41
36:e:132:LYS:HD2	36:e:132:LYS:HA	1.79	0.41
46:p:77:THR:HB	46:p:102:ARG:HG3	2.01	0.41
49:s:118:LEU:HD23	49:s:118:LEU:HA	1.88	0.41
52:v:51:ARG:HA	62:v:101:PNS:H422	2.02	0.41
53:w:129:GLU:HG3	53:w:151:LYS:HD3	2.01	0.41
54:A:2940:A:OP1	58:C:77:LYS:HG2	2.20	0.41
6:J:114:LEU:HD23	6:J:114:LEU:HA	1.93	0.41
17:U:9:LEU:HA	17:U:9:LEU:HD12	1.79	0.41
18:V:129:LYS:HB3	18:V:149:ARG:HH22	1.85	0.41
28:6:60:ARG:HA	28:6:60:ARG:HD2	1.74	0.41
45:o:12:ILE:HG21	45:o:16:GLN:HA	2.02	0.41
4:H:75:ARG:HH21	20:X:100:ARG:HH22	1.68	0.41
6:J:25:ARG:H	6:J:25:ARG:HG3	1.73	0.41
12:P:63:ARG:HG3	12:P:177:ARG:HH11	1.86	0.41
15:S:74:ARG:HE	15:S:74:ARG:HB2	1.62	0.41
17:U:35:GLN:NE2	54:A:2372:U:O4	2.40	0.41
19:W:117:ILE:HD13	19:W:117:ILE:HA	1.85	0.41
20:X:8:VAL:HG21	21:Y:210:ARG:NH1	2.36	0.41
23:0:90:ASN:OD1	23:0:93:ARG:NH2	2.46	0.41
28:6:27:ARG:N	54:A:2073:A:OP2	2.54	0.41
29:7:113:TRP:HH2	29:7:120:THR:HG23	1.85	0.41
35:d:150:LEU:HD13	35:d:150:LEU:HA	1.87	0.41
36:e:172:ILE:HD12	36:e:172:ILE:HA	1.91	0.41
37:f:101:THR:OG1	37:f:102:LEU:N	2.54	0.41
39:h:157:SER:O	39:h:157:SER:OG	2.29	0.41
40:i:88:LEU:HD23	40:i:117:LEU:HB2	2.03	0.41
48:r:64:PRO:HD2	48:r:75:TRP:HA	2.03	0.41
54:A:2171:U:C2	54:A:2173:G:H4'	2.56	0.41
54:A:2628:U:H5''	54:A:2629:A:H3'	2.03	0.41
54:A:3064:A:H2'	54:A:3101:A:N6	2.36	0.41
1:D:121:PRO:HB3	1:D:166:SER:HA	2.03	0.41
2:E:328:LEU:HD23	2:E:328:LEU:HA	1.86	0.41
5:I:51:THR:O	10:N:250:ARG:NH2	2.54	0.41
12:P:45:ALA:N	28:6:225:LEU:O	2.41	0.41
13:Q:224:MET:HE3	13:Q:243:ILE:HD12	2.01	0.41
15:S:100:HIS:HB2	15:S:134:LEU:HD21	2.03	0.41
20:X:208:LEU:HD13	20:X:212:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:5:300:ARG:HG2	54:A:2390:A:H5'	2.02	0.41
28:6:140:GLU:HA	28:6:144:GLY:HA3	2.02	0.41
30:8:136:ILE:HD12	30:8:136:ILE:HA	1.91	0.41
55:B:1621:A:H61	55:B:1645:A:H3'	1.86	0.41
59:G:142:PHE:HD2	59:G:182:VAL:HG23	1.86	0.41
1:D:223:THR:HG21	1:D:235:GLN:HE21	1.85	0.40
1:D:237:LEU:HD23	1:D:237:LEU:HA	1.89	0.40
9:M:254:LYS:O	9:M:258:THR:HG23	2.21	0.40
13:Q:236:PRO:HG3	13:Q:261:ASN:HA	2.03	0.40
14:R:98:ASN:HD22	54:A:2147:G:H4'	1.86	0.40
15:S:171:ILE:HD13	54:A:2143:G:H4'	2.02	0.40
19:W:139:GLU:CD	19:W:139:GLU:H	2.29	0.40
21:Y:165:PRO:HB2	21:Y:181:PHE:HD2	1.85	0.40
27:5:147:ILE:HG13	27:5:150:GLN:HB3	2.03	0.40
34:c:83:PHE:CG	34:c:88:LEU:HD22	2.56	0.40
58:C:74:ALA:O	58:C:78:THR:OG1	2.29	0.40
12:P:155:SER:HB2	55:B:1639:U:H5''	2.03	0.40
23:0:180:LYS:H	23:0:180:LYS:HG3	1.70	0.40
24:1:16:ILE:HD12	24:1:36:ARG:HA	2.03	0.40
29:7:154:ILE:HG22	29:7:164:VAL:HG21	2.02	0.40
53:w:144:ILE:H	53:w:144:ILE:HG13	1.64	0.40
54:A:2138:U:O2'	54:A:2151:A:N3	2.52	0.40
54:A:2576:A:N6	58:C:136:LYS:HD3	2.36	0.40
2:E:160:SER:HA	2:E:163:GLU:HG2	2.03	0.40
5:I:139:LYS:HB2	5:I:139:LYS:HE2	1.78	0.40
7:K:51:SER:O	16:T:206:ARG:NH1	2.55	0.40
15:S:163:LYS:HB2	33:b:106:ASP:HB3	2.04	0.40
23:0:179:ARG:NH1	23:0:182:PRO:HG3	2.37	0.40
27:5:165:GLN:HE22	27:5:175:THR:HG22	1.85	0.40
27:5:204:VAL:HG13	49:s:152:GLN:NE2	2.36	0.40
28:6:183:ASP:OD2	28:6:183:ASP:N	2.55	0.40
36:e:255:VAL:HG13	36:e:259:GLU:HB2	2.03	0.40
38:g:94:ILE:HD11	38:g:162:LEU:HG	2.03	0.40
39:h:71:GLU:HG3	39:h:86:TRP:CE2	2.57	0.40
42:k:17:ARG:HA	42:k:52:ILE:HG23	2.03	0.40
42:k:74:LEU:HD11	48:r:49:ILE:HD11	2.03	0.40
48:r:104:ILE:HD13	48:r:104:ILE:HA	1.92	0.40
54:A:2127:A:H4'	54:A:2251:A:C5	2.56	0.40
55:B:1667:C:H2'	55:B:1668:U:C6	2.56	0.40
2:E:52:HIS:O	11:O:146:ASN:ND2	2.38	0.40
11:O:47:ALA:HB3	54:A:2455:U:H5''	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:P:65:GLU:OE2	28:6:74:TYR:OH	2.35	0.40
14:R:31:PHE:HB3	14:R:35:LYS:HE2	2.02	0.40
27:5:133:PRO:HG3	27:5:239:ILE:HD13	2.02	0.40
27:5:301:PRO:HD3	54:A:2390:A:H4'	2.03	0.40
35:d:267:PRO:HB2	35:d:269:TRP:CD1	2.57	0.40
37:f:106:TYR:CZ	37:f:178:LEU:HD23	2.57	0.40
52:v:65:LYS:HD2	52:v:65:LYS:HA	1.79	0.40
54:A:3041:U:H2'	54:A:3042:U:C6	2.56	0.40
1:D:166:SER:OG	1:D:167:ASN:N	2.53	0.40
2:E:177:LYS:HB3	2:E:298:LYS:HD2	2.04	0.40
6:J:48:GLN:OE1	6:J:48:GLN:N	2.55	0.40
14:R:122:ARG:HD3	32:a:36:TYR:HE2	1.86	0.40
14:R:148:TYR:OH	15:S:146:LYS:O	2.38	0.40
28:6:263:SER:HB3	28:6:342:PHE:CD2	2.56	0.40
36:e:48:LEU:HD22	36:e:175:GLN:HB3	2.04	0.40
38:g:88:ARG:NH1	38:g:92:HIS:O	2.55	0.40
49:s:96:GLN:NE2	49:s:301:LEU:O	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	234/305 (77%)	219 (94%)	14 (6%)	1 (0%)	30	60
2	E	302/348 (87%)	284 (94%)	18 (6%)	0	100	100
3	F	248/311 (80%)	240 (97%)	8 (3%)	0	100	100
4	H	93/267 (35%)	86 (92%)	7 (8%)	0	100	100
5	I	154/261 (59%)	135 (88%)	19 (12%)	0	100	100
6	J	138/192 (72%)	127 (92%)	11 (8%)	0	100	100
7	K	175/178 (98%)	165 (94%)	10 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	L	113/145 (78%)	102 (90%)	11 (10%)	0	100	100
9	M	285/296 (96%)	267 (94%)	18 (6%)	0	100	100
10	N	203/251 (81%)	193 (95%)	9 (4%)	1 (0%)	24	55
11	O	150/175 (86%)	144 (96%)	6 (4%)	0	100	100
12	P	139/179 (78%)	129 (93%)	10 (7%)	0	100	100
13	Q	215/292 (74%)	202 (94%)	13 (6%)	0	100	100
14	R	138/149 (93%)	136 (99%)	2 (1%)	0	100	100
15	S	154/205 (75%)	148 (96%)	6 (4%)	0	100	100
16	T	164/212 (77%)	156 (95%)	8 (5%)	0	100	100
17	U	148/153 (97%)	132 (89%)	14 (10%)	2 (1%)	9	33
18	V	200/216 (93%)	187 (94%)	13 (6%)	0	100	100
19	W	107/148 (72%)	104 (97%)	3 (3%)	0	100	100
20	X	241/256 (94%)	231 (96%)	10 (4%)	0	100	100
21	Y	174/250 (70%)	170 (98%)	4 (2%)	0	100	100
22	Z	118/161 (73%)	113 (96%)	5 (4%)	0	100	100
23	0	106/188 (56%)	104 (98%)	2 (2%)	0	100	100
24	1	50/65 (77%)	48 (96%)	2 (4%)	0	100	100
25	2	43/92 (47%)	42 (98%)	1 (2%)	0	100	100
26	3	93/188 (50%)	88 (95%)	5 (5%)	0	100	100
27	5	383/423 (90%)	361 (94%)	22 (6%)	0	100	100
28	6	316/380 (83%)	293 (93%)	23 (7%)	0	100	100
29	7	285/338 (84%)	267 (94%)	17 (6%)	1 (0%)	30	60
30	8	108/206 (52%)	86 (80%)	19 (18%)	3 (3%)	4	21
31	9	113/137 (82%)	106 (94%)	7 (6%)	0	100	100
32	a	78/142 (55%)	74 (95%)	4 (5%)	0	100	100
33	b	146/155 (94%)	133 (91%)	13 (9%)	0	100	100
34	c	271/332 (82%)	263 (97%)	8 (3%)	0	100	100
35	d	203/306 (66%)	189 (93%)	14 (7%)	0	100	100
36	e	211/279 (76%)	189 (90%)	22 (10%)	0	100	100
37	f	110/194 (57%)	95 (86%)	15 (14%)	0	100	100
38	g	127/166 (76%)	119 (94%)	8 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	h	96/158 (61%)	92 (96%)	4 (4%)	0	100	100
40	i	95/128 (74%)	90 (95%)	5 (5%)	0	100	100
41	j	83/123 (68%)	79 (95%)	4 (5%)	0	100	100
42	k	76/112 (68%)	68 (90%)	8 (10%)	0	100	100
43	l	21/138 (15%)	19 (90%)	2 (10%)	0	100	100
44	m	43/128 (34%)	34 (79%)	9 (21%)	0	100	100
45	o	89/102 (87%)	86 (97%)	3 (3%)	0	100	100
46	p	119/206 (58%)	115 (97%)	4 (3%)	0	100	100
47	q	126/222 (57%)	121 (96%)	5 (4%)	0	100	100
48	r	140/196 (71%)	133 (95%)	7 (5%)	0	100	100
49	s	366/439 (83%)	347 (95%)	19 (5%)	0	100	100
51	u	109/234 (47%)	99 (91%)	10 (9%)	0	100	100
52	v	67/70 (96%)	63 (94%)	4 (6%)	0	100	100
53	w	77/156 (49%)	66 (86%)	11 (14%)	0	100	100
57	Y2	2/29 (7%)	0	2 (100%)	0	100	100
58	C	112/166 (68%)	96 (86%)	15 (13%)	1 (1%)	14	43
59	G	92/240 (38%)	60 (65%)	28 (30%)	4 (4%)	2	14
All	All	8249/11388 (72%)	7695 (93%)	541 (7%)	13 (0%)	44	71

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	207	ILE
17	U	118	PRO
30	8	186	GLN
30	8	187	PRO
30	8	188	PRO
59	G	149	LYS
17	U	117	SER
59	G	190	LEU
10	N	48	PRO
59	G	171	ASN
59	G	189	ASP
29	7	291	PRO
58	C	88	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	190/245 (78%)	172 (90%)	18 (10%)	8	29
2	E	259/290 (89%)	235 (91%)	24 (9%)	8	30
3	F	217/262 (83%)	193 (89%)	24 (11%)	6	22
4	H	86/228 (38%)	77 (90%)	9 (10%)	6	25
5	I	145/232 (62%)	135 (93%)	10 (7%)	14	41
6	J	113/150 (75%)	98 (87%)	15 (13%)	4	17
7	K	155/156 (99%)	145 (94%)	10 (6%)	15	43
8	L	98/124 (79%)	86 (88%)	12 (12%)	5	19
9	M	245/249 (98%)	223 (91%)	22 (9%)	9	31
10	N	172/211 (82%)	156 (91%)	16 (9%)	8	30
11	O	133/150 (89%)	123 (92%)	10 (8%)	12	38
12	P	123/154 (80%)	110 (89%)	13 (11%)	6	24
13	Q	199/256 (78%)	177 (89%)	22 (11%)	6	22
14	R	118/126 (94%)	108 (92%)	10 (8%)	10	33
15	S	141/180 (78%)	124 (88%)	17 (12%)	5	20
16	T	146/182 (80%)	138 (94%)	8 (6%)	19	48
17	U	124/135 (92%)	114 (92%)	10 (8%)	11	36
18	V	172/191 (90%)	144 (84%)	28 (16%)	2	11
19	W	89/119 (75%)	78 (88%)	11 (12%)	4	19
20	X	219/229 (96%)	199 (91%)	20 (9%)	9	31
21	Y	159/223 (71%)	145 (91%)	14 (9%)	9	32
22	Z	111/147 (76%)	103 (93%)	8 (7%)	13	40
23	0	97/164 (59%)	85 (88%)	12 (12%)	4	19
24	1	49/60 (82%)	43 (88%)	6 (12%)	5	19
25	2	39/72 (54%)	36 (92%)	3 (8%)	12	37
26	3	88/166 (53%)	78 (89%)	10 (11%)	5	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	5	348/368 (95%)	308 (88%)	40 (12%)	5	21
28	6	265/332 (80%)	231 (87%)	34 (13%)	4	18
29	7	263/303 (87%)	231 (88%)	32 (12%)	5	19
30	8	91/190 (48%)	81 (89%)	10 (11%)	6	23
31	9	99/112 (88%)	94 (95%)	5 (5%)	21	50
32	a	78/133 (59%)	72 (92%)	6 (8%)	12	37
33	b	130/135 (96%)	113 (87%)	17 (13%)	4	17
34	c	241/288 (84%)	220 (91%)	21 (9%)	9	32
35	d	193/274 (70%)	175 (91%)	18 (9%)	8	30
36	e	188/236 (80%)	174 (93%)	14 (7%)	13	38
37	f	101/173 (58%)	88 (87%)	13 (13%)	4	17
38	g	119/148 (80%)	109 (92%)	10 (8%)	10	34
39	h	95/148 (64%)	83 (87%)	12 (13%)	4	18
40	i	86/110 (78%)	73 (85%)	13 (15%)	3	13
41	j	68/97 (70%)	64 (94%)	4 (6%)	18	46
42	k	71/90 (79%)	63 (89%)	8 (11%)	5	21
43	l	23/116 (20%)	22 (96%)	1 (4%)	26	54
44	m	40/113 (35%)	36 (90%)	4 (10%)	7	27
45	o	78/87 (90%)	68 (87%)	10 (13%)	4	18
46	p	117/181 (65%)	105 (90%)	12 (10%)	7	25
47	q	110/178 (62%)	97 (88%)	13 (12%)	5	20
48	r	133/169 (79%)	120 (90%)	13 (10%)	7	28
49	s	326/381 (86%)	291 (89%)	35 (11%)	6	24
51	u	105/200 (52%)	92 (88%)	13 (12%)	4	19
52	v	59/60 (98%)	51 (86%)	8 (14%)	3	16
53	w	73/136 (54%)	63 (86%)	10 (14%)	3	16
57	Y2	3/3 (100%)	2 (67%)	1 (33%)	0	1
58	C	102/146 (70%)	90 (88%)	12 (12%)	5	20
59	G	90/221 (41%)	76 (84%)	14 (16%)	2	12
All	All	7382/9829 (75%)	6617 (90%)	765 (10%)	9	25

All (765) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	64	VAL
1	D	74	ILE
1	D	79	MET
1	D	115	GLU
1	D	130	ARG
1	D	163	ILE
1	D	171	ARG
1	D	177	ARG
1	D	219	LYS
1	D	220	VAL
1	D	221	ASN
1	D	223	THR
1	D	232	ARG
1	D	236	VAL
1	D	243	THR
1	D	244	VAL
1	D	247	VAL
1	D	251	ASP
2	E	65	VAL
2	E	97	VAL
2	E	113	ASP
2	E	119	VAL
2	E	120	THR
2	E	142	MET
2	E	144	THR
2	E	145	LEU
2	E	152	VAL
2	E	168	LEU
2	E	181	ILE
2	E	184	ASN
2	E	204	VAL
2	E	207	THR
2	E	209	LYS
2	E	218	VAL
2	E	248	ILE
2	E	289	VAL
2	E	296	LEU
2	E	297	VAL
2	E	299	VAL
2	E	327	GLU
2	E	331	ASP
2	E	345	ILE
3	F	45	GLU

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Mol	Chain	Res	Type
3	F	51	VAL
3	F	55	VAL
3	F	57	THR
3	F	89	THR
3	F	96	LEU
3	F	110	SER
3	F	137	ARG
3	F	140	SER
3	F	143	SER
3	F	145	LEU
3	F	159	THR
3	F	187	LEU
3	F	195	LEU
3	F	197	THR
3	F	214	ASP
3	F	222	THR
3	F	232	GLU
3	F	235	SER
3	F	239	THR
3	F	258	THR
3	F	274	LEU
3	F	277	ASP
3	F	287	SER
4	H	53	THR
4	H	54	VAL
4	H	83	VAL
4	H	86	THR
4	H	94	LEU
4	H	111	LEU
4	H	114	VAL
4	H	145	LEU
4	H	147	ARG
5	I	60	ILE
5	I	63	SER
5	I	125	VAL
5	I	129	GLN
5	I	130	VAL
5	I	134	PHE
5	I	152	MET
5	I	161	VAL
5	I	171	VAL
5	I	197	LEU

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Mol	Chain	Res	Type
6	J	46	ILE
6	J	47	ASN
6	J	57	THR
6	J	68	THR
6	J	72	VAL
6	J	76	ARG
6	J	77	THR
6	J	86	THR
6	J	87	VAL
6	J	106	LYS
6	J	119	GLU
6	J	137	LEU
6	J	138	SER
6	J	153	ILE
6	J	156	VAL
7	K	20	LEU
7	K	21	LEU
7	K	62	THR
7	K	78	SER
7	K	81	THR
7	K	94	GLN
7	K	101	VAL
7	K	120	THR
7	K	127	LEU
7	K	153	LYS
8	L	36	THR
8	L	38	VAL
8	L	42	ASP
8	L	46	LEU
8	L	85	LEU
8	L	96	MET
8	L	105	VAL
8	L	108	ILE
8	L	111	ASN
8	L	135	SER
8	L	140	ILE
8	L	143	ASN
9	M	14	ASP
9	M	39	ARG
9	M	62	ARG
9	M	84	ASN
9	M	97	SER

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Mol	Chain	Res	Type
9	M	127	VAL
9	M	129	ILE
9	M	132	LEU
9	M	141	VAL
9	M	155	GLU
9	M	156	VAL
9	M	162	LEU
9	M	182	ARG
9	M	187	VAL
9	M	203	ARG
9	M	244	LEU
9	M	246	ASP
9	M	248	THR
9	M	251	GLU
9	M	261	ASP
9	M	274	VAL
9	M	286	THR
10	N	58	LEU
10	N	59	VAL
10	N	62	VAL
10	N	77	THR
10	N	80	THR
10	N	83	THR
10	N	112	SER
10	N	121	ILE
10	N	124	VAL
10	N	131	ILE
10	N	151	VAL
10	N	177	ASP
10	N	191	SER
10	N	204	GLU
10	N	224	LEU
10	N	247	MET
11	O	17	ARG
11	O	20	LEU
11	O	33	LEU
11	O	59	LEU
11	O	67	ASP
11	O	105	THR
11	O	113	ARG
11	O	114	SER
11	O	122	VAL

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Mol	Chain	Res	Type
11	O	155	ASP
12	P	42	GLU
12	P	56	LEU
12	P	71	VAL
12	P	75	ARG
12	P	83	VAL
12	P	95	GLU
12	P	103	VAL
12	P	107	THR
12	P	121	ASN
12	P	134	GLN
12	P	155	SER
12	P	157	SER
12	P	166	THR
13	Q	86	ARG
13	Q	105	VAL
13	Q	113	VAL
13	Q	119	VAL
13	Q	123	ASP
13	Q	134	LEU
13	Q	141	SER
13	Q	143	ARG
13	Q	150	ILE
13	Q	154	VAL
13	Q	155	ILE
13	Q	160	VAL
13	Q	171	VAL
13	Q	174	ILE
13	Q	184	ASP
13	Q	209	GLN
13	Q	215	VAL
13	Q	219	GLU
13	Q	224	MET
13	Q	240	ILE
13	Q	247	LEU
13	Q	265	LEU
14	R	10	LEU
14	R	11	ARG
14	R	13	ARG
14	R	35	LYS
14	R	36	ASN
14	R	66	THR

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Mol	Chain	Res	Type
14	R	67	LEU
14	R	87	ILE
14	R	119	LEU
14	R	132	LEU
15	S	54	THR
15	S	70	VAL
15	S	76	HIS
15	S	78	GLU
15	S	99	VAL
15	S	108	VAL
15	S	126	GLU
15	S	131	GLU
15	S	133	VAL
15	S	134	LEU
15	S	143	LEU
15	S	144	LEU
15	S	164	THR
15	S	182	LYS
15	S	188	THR
15	S	191	THR
15	S	195	ILE
16	T	84	LYS
16	T	87	MET
16	T	93	LEU
16	T	97	MET
16	T	142	ILE
16	T	170	VAL
16	T	207	THR
16	T	209	VAL
17	U	12	LEU
17	U	19	VAL
17	U	24	PHE
17	U	25	PHE
17	U	26	ILE
17	U	28	LEU
17	U	53	LEU
17	U	79	ARG
17	U	106	THR
17	U	131	GLU
18	V	20	ARG
18	V	28	SER
18	V	39	ILE

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Mol	Chain	Res	Type
18	V	45	VAL
18	V	47	GLU
18	V	56	LEU
18	V	61	THR
18	V	64	ILE
18	V	69	ASP
18	V	79	VAL
18	V	85	TRP
18	V	86	VAL
18	V	87	VAL
18	V	107	THR
18	V	120	VAL
18	V	122	LEU
18	V	124	ASP
18	V	131	THR
18	V	133	ILE
18	V	144	VAL
18	V	154	ILE
18	V	169	THR
18	V	177	THR
18	V	183	LEU
18	V	186	THR
18	V	193	THR
18	V	204	ILE
18	V	207	THR
19	W	49	ARG
19	W	54	LYS
19	W	57	GLU
19	W	69	THR
19	W	83	VAL
19	W	88	CYS
19	W	105	VAL
19	W	117	ILE
19	W	125	VAL
19	W	129	THR
19	W	141	THR
20	X	10	LEU
20	X	21	CYS
20	X	39	THR
20	X	52	ILE
20	X	56	ASN
20	X	62	VAL

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Mol	Chain	Res	Type
20	X	64	ASP
20	X	75	SER
20	X	100	ARG
20	X	101	LEU
20	X	125	VAL
20	X	127	VAL
20	X	128	THR
20	X	142	ASP
20	X	152	ASP
20	X	208	LEU
20	X	216	ARG
20	X	218	LEU
20	X	220	GLU
20	X	243	LEU
21	Y	69	ASP
21	Y	86	THR
21	Y	97	ASP
21	Y	128	SER
21	Y	131	ARG
21	Y	140	ASP
21	Y	153	LEU
21	Y	158	THR
21	Y	160	GLN
21	Y	172	ILE
21	Y	190	LEU
21	Y	198	ARG
21	Y	216	ARG
21	Y	226	LEU
22	Z	70	THR
22	Z	71	ARG
22	Z	74	SER
22	Z	110	LEU
22	Z	123	LYS
22	Z	124	LEU
22	Z	142	THR
22	Z	154	VAL
23	0	84	ARG
23	0	86	THR
23	0	89	VAL
23	0	104	LYS
23	0	106	ASN
23	0	108	ASP

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Mol	Chain	Res	Type
23	0	116	LEU
23	0	156	THR
23	0	157	VAL
23	0	166	SER
23	0	175	ILE
23	0	180	LYS
24	1	16	ILE
24	1	17	LEU
24	1	26	THR
24	1	44	LEU
24	1	55	LEU
24	1	58	GLU
25	2	58	ILE
25	2	72	THR
25	2	84	LEU
26	3	104	ARG
26	3	111	ILE
26	3	112	ASP
26	3	137	THR
26	3	148	VAL
26	3	157	LEU
26	3	164	SER
26	3	168	ARG
26	3	174	ASP
26	3	188	VAL
27	5	55	LEU
27	5	67	VAL
27	5	86	ARG
27	5	98	LEU
27	5	126	THR
27	5	147	ILE
27	5	155	LEU
27	5	165	GLN
27	5	166	THR
27	5	175	THR
27	5	180	ILE
27	5	182	ASP
27	5	187	LEU
27	5	212	THR
27	5	218	LEU
27	5	233	LYS
27	5	236	LEU

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Mol	Chain	Res	Type
27	5	238	THR
27	5	243	GLU
27	5	246	GLU
27	5	253	LEU
27	5	262	ILE
27	5	273	VAL
27	5	295	ASP
27	5	304	LEU
27	5	315	LEU
27	5	340	VAL
27	5	344	SER
27	5	351	VAL
27	5	355	LEU
27	5	360	ASN
27	5	361	THR
27	5	364	LEU
27	5	370	VAL
27	5	373	LEU
27	5	378	SER
27	5	381	LEU
27	5	404	VAL
27	5	409	GLU
27	5	415	LEU
28	6	53	SER
28	6	127	THR
28	6	132	LEU
28	6	140	GLU
28	6	157	LEU
28	6	161	LEU
28	6	163	HIS
28	6	166	THR
28	6	171	VAL
28	6	173	LEU
28	6	184	LEU
28	6	209	GLU
28	6	215	THR
28	6	219	THR
28	6	221	LEU
28	6	222	ASP
28	6	226	LEU
28	6	231	GLU
28	6	233	LEU

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Mol	Chain	Res	Type
28	6	238	THR
28	6	268	LEU
28	6	298	PHE
28	6	310	THR
28	6	316	LEU
28	6	323	TRP
28	6	324	ASP
28	6	325	ASP
28	6	328	THR
28	6	333	GLN
28	6	334	LEU
28	6	341	VAL
28	6	364	ARG
28	6	371	ASP
28	6	376	THR
29	7	38	THR
29	7	40	LEU
29	7	54	ARG
29	7	57	SER
29	7	65	ILE
29	7	67	VAL
29	7	73	THR
29	7	80	VAL
29	7	96	SER
29	7	107	LEU
29	7	114	ASP
29	7	125	ILE
29	7	126	LYS
29	7	143	TRP
29	7	163	MET
29	7	164	VAL
29	7	166	LEU
29	7	167	VAL
29	7	180	CYS
29	7	183	VAL
29	7	209	LEU
29	7	210	ILE
29	7	216	PHE
29	7	228	GLU
29	7	237	VAL
29	7	257	ILE
29	7	280	VAL

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Mol	Chain	Res	Type
29	7	281	SER
29	7	294	ILE
29	7	304	VAL
29	7	314	ASP
29	7	322	LYS
30	8	85	ILE
30	8	92	LEU
30	8	104	VAL
30	8	107	THR
30	8	109	GLU
30	8	111	THR
30	8	116	LEU
30	8	134	ASP
30	8	137	ARG
30	8	149	GLU
31	9	19	SER
31	9	41	ILE
31	9	45	THR
31	9	96	VAL
31	9	122	THR
32	a	42	ASP
32	a	57	THR
32	a	60	CYS
32	a	65	VAL
32	a	66	ASP
32	a	122	ARG
33	b	26	LEU
33	b	27	GLN
33	b	30	SER
33	b	40	SER
33	b	51	VAL
33	b	58	ASN
33	b	62	VAL
33	b	75	VAL
33	b	81	ASN
33	b	87	GLU
33	b	94	VAL
33	b	103	LYS
33	b	122	ASP
33	b	134	THR
33	b	139	THR
33	b	148	VAL

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Mol	Chain	Res	Type
33	b	149	GLN
34	c	51	LEU
34	c	72	ILE
34	c	85	LEU
34	c	96	CYS
34	c	98	ILE
34	c	100	SER
34	c	102	GLU
34	c	133	SER
34	c	135	THR
34	c	136	CYS
34	c	158	ASP
34	c	163	GLU
34	c	165	VAL
34	c	166	VAL
34	c	206	SER
34	c	219	LEU
34	c	241	LEU
34	c	245	LEU
34	c	248	ARG
34	c	280	LEU
34	c	308	THR
35	d	81	THR
35	d	84	ILE
35	d	89	VAL
35	d	127	ASP
35	d	150	LEU
35	d	158	ASP
35	d	162	THR
35	d	164	VAL
35	d	173	THR
35	d	192	SER
35	d	195	VAL
35	d	208	VAL
35	d	221	THR
35	d	241	ASP
35	d	246	VAL
35	d	249	GLU
35	d	252	LEU
35	d	266	VAL
36	e	82	SER
36	e	86	ASP

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Mol	Chain	Res	Type
36	e	129	LEU
36	e	138	THR
36	e	143	LYS
36	e	156	ASN
36	e	158	VAL
36	e	172	ILE
36	e	197	GLU
36	e	214	THR
36	e	240	THR
36	e	248	ASN
36	e	251	HIS
36	e	252	HIS
37	f	62	LEU
37	f	63	ILE
37	f	88	TYR
37	f	90	VAL
37	f	99	ASP
37	f	104	GLU
37	f	113	LEU
37	f	131	THR
37	f	151	THR
37	f	152	THR
37	f	160	SER
37	f	169	ILE
37	f	182	VAL
38	g	44	GLU
38	g	55	THR
38	g	56	ARG
38	g	57	ILE
38	g	89	SER
38	g	100	ILE
38	g	108	THR
38	g	109	VAL
38	g	111	ARG
38	g	164	LYS
39	h	66	LEU
39	h	71	GLU
39	h	77	VAL
39	h	88	ASP
39	h	94	SER
39	h	96	LEU
39	h	111	VAL

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Mol	Chain	Res	Type
39	h	121	CYS
39	h	152	LEU
39	h	155	THR
39	h	156	TRP
39	h	157	SER
40	i	32	ILE
40	i	34	ILE
40	i	44	VAL
40	i	62	ILE
40	i	63	LEU
40	i	73	LEU
40	i	74	ILE
40	i	80	LEU
40	i	87	GLU
40	i	88	LEU
40	i	98	VAL
40	i	102	MET
40	i	128	ARG
41	j	81	SER
41	j	83	GLU
41	j	92	GLN
41	j	98	LEU
42	k	13	VAL
42	k	30	THR
42	k	45	THR
42	k	49	CYS
42	k	52	ILE
42	k	55	VAL
42	k	66	VAL
42	k	84	LEU
43	l	136	LYS
44	m	42	ARG
44	m	54	VAL
44	m	58	LYS
44	m	66	ILE
45	o	28	SER
45	o	29	LEU
45	o	35	MET
45	o	37	ARG
45	o	59	GLU
45	o	65	VAL
45	o	74	ILE

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Mol	Chain	Res	Type
45	o	82	PHE
45	o	90	ASP
45	o	100	LYS
46	p	41	SER
46	p	52	SER
46	p	56	ASP
46	p	57	THR
46	p	96	ASN
46	p	107	THR
46	p	111	ILE
46	p	125	ASN
46	p	135	LEU
46	p	137	SER
46	p	144	PHE
46	p	149	ASP
47	q	41	ASP
47	q	52	LEU
47	q	68	SER
47	q	70	VAL
47	q	71	VAL
47	q	85	LEU
47	q	95	SER
47	q	96	LEU
47	q	99	MET
47	q	108	LEU
47	q	114	ARG
47	q	117	ARG
47	q	131	MET
48	r	41	THR
48	r	53	ILE
48	r	54	THR
48	r	70	CYS
48	r	77	LEU
48	r	85	ASP
48	r	102	ARG
48	r	149	ARG
48	r	152	THR
48	r	159	VAL
48	r	183	ASP
48	r	186	CYS
48	r	193	LYS
49	s	48	VAL

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Mol	Chain	Res	Type
49	s	66	TRP
49	s	74	GLU
49	s	92	MET
49	s	112	THR
49	s	116	SER
49	s	142	LEU
49	s	177	LEU
49	s	182	SER
49	s	195	LEU
49	s	200	LEU
49	s	229	LEU
49	s	251	VAL
49	s	263	THR
49	s	275	LYS
49	s	284	VAL
49	s	288	THR
49	s	304	ASP
49	s	306	LEU
49	s	321	GLU
49	s	353	ARG
49	s	356	VAL
49	s	360	VAL
49	s	361	ILE
49	s	374	LEU
49	s	376	THR
49	s	379	LEU
49	s	381	THR
49	s	392	ILE
49	s	406	GLU
49	s	410	VAL
49	s	415	ASP
49	s	418	LEU
49	s	419	LEU
49	s	424	PHE
51	u	93	ASP
51	u	96	MET
51	u	100	LEU
51	u	104	GLU
51	u	111	VAL
51	u	119	ARG
51	u	154	ASP
51	u	166	ASP

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Mol	Chain	Res	Type
51	u	170	VAL
51	u	176	VAL
51	u	184	THR
51	u	193	LEU
51	u	196	LEU
52	v	5	SER
52	v	9	VAL
52	v	17	LEU
52	v	26	THR
52	v	27	ASP
52	v	57	LYS
52	v	63	ASN
52	v	70	ILE
53	w	74	LEU
53	w	112	SER
53	w	115	GLN
53	w	126	PHE
53	w	132	ASP
53	w	133	ILE
53	w	136	GLU
53	w	142	GLN
53	w	148	ILE
53	w	150	ASP
57	Y2	26	LYS
58	C	53	LEU
58	C	78	THR
58	C	92	VAL
58	C	95	CYS
58	C	109[A]	ARG
58	C	109[B]	ARG
58	C	123	GLU
58	C	132	ARG
58	C	133	GLU
58	C	136	LYS
58	C	148	THR
58	C	155	LEU
59	G	134	ASP
59	G	135	LEU
59	G	146	VAL
59	G	148	LEU
59	G	160	GLU
59	G	170	LEU

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Mol	Chain	Res	Type
59	G	174	LYS
59	G	182	VAL
59	G	186	ASP
59	G	202	THR
59	G	203	VAL
59	G	204	MET
59	G	210	LYS
59	G	217	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (136) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	165	ASN
1	D	235	GLN
2	E	57	ASN
2	E	115	GLN
2	E	117	HIS
2	E	128	HIS
2	E	139	ASN
2	E	231	HIS
3	F	58	HIS
3	F	105	ASN
3	F	184	GLN
4	H	104	ASN
4	H	126	GLN
5	I	43	GLN
5	I	101	ASN
5	I	119	HIS
5	I	141	GLN
5	I	189	GLN
5	I	193	ASN
7	K	56	HIS
7	K	70	ASN
7	K	89	GLN
8	L	43	ASN
8	L	80	GLN
8	L	104	ASN
8	L	143	ASN
9	M	58	GLN
10	N	86	ASN
10	N	178	GLN
11	O	69	ASN

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Mol	Chain	Res	Type
11	O	150	GLN
12	P	50	ASN
12	P	97	GLN
13	Q	93	GLN
13	Q	158	GLN
13	Q	172	GLN
13	Q	175	GLN
14	R	22	GLN
14	R	30	HIS
14	R	79	HIS
15	S	140	ASN
16	T	62	GLN
16	T	101	GLN
17	U	4	ASN
17	U	55	ASN
17	U	74	HIS
17	U	82	HIS
18	V	92	ASN
19	W	51	GLN
19	W	80	HIS
20	X	27	HIS
20	X	93	ASN
20	X	241	GLN
21	Y	88	GLN
21	Y	122	GLN
21	Y	147	GLN
21	Y	160	GLN
21	Y	195	ASN
21	Y	225	ASN
22	Z	47	GLN
22	Z	107	ASN
23	0	170	GLN
25	2	57	ASN
27	5	146	HIS
27	5	165	GLN
27	5	324	GLN
28	6	69	HIS
28	6	307	HIS
28	6	354	GLN
28	6	359	HIS
29	7	45	ASN
29	7	69	HIS

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Mol	Chain	Res	Type
29	7	84	ASN
29	7	94	HIS
29	7	247	ASN
29	7	285	ASN
29	7	287	GLN
30	8	143	GLN
32	a	44	ASN
33	b	27	GLN
33	b	102	GLN
33	b	123	ASN
33	b	129	GLN
33	b	149	GLN
34	c	82	ASN
34	c	122	ASN
34	c	123	GLN
34	c	128	GLN
34	c	139	GLN
34	c	155	ASN
34	c	168	HIS
35	d	161	HIS
35	d	217	HIS
35	d	274	GLN
36	e	95	ASN
36	e	168	GLN
36	e	248	ASN
36	e	251	HIS
36	e	252	HIS
37	f	61	HIS
37	f	81	ASN
37	f	92	ASN
37	f	115	ASN
39	h	99	ASN
39	h	110	HIS
39	h	118	HIS
39	h	119	GLN
40	i	59	ASN
40	i	65	ASN
44	m	59	GLN
46	p	163	GLN
47	q	120	HIS
47	q	138	GLN
47	q	142	ASN

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Mol	Chain	Res	Type
47	q	147	GLN
48	r	62	ASN
48	r	109	GLN
48	r	112	HIS
48	r	184	ASN
49	s	107	GLN
49	s	207	HIS
49	s	327	ASN
49	s	387	ASN
49	s	408	ASN
49	s	423	HIS
49	s	427	ASN
51	u	105	ASN
51	u	156	HIS
53	w	142	GLN
58	C	63	GLN
58	C	97	GLN
58	C	128	HIS
58	C	139	GLN
59	G	131	ASN
59	G	140	GLN
59	G	171	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
54	A	1443/1559 (92%)	421 (29%)	22 (1%)
55	B	51/73 (69%)	23 (45%)	1 (1%)
56	24	73/73 (100%)	37 (50%)	1 (1%)
All	All	1567/1705 (91%)	481 (30%)	24 (1%)

All (481) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
54	A	1674	A
54	A	1676	A
54	A	1677	C
54	A	1678	C
54	A	1679	U
54	A	1680	A
54	A	1681	G

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Mol	Chain	Res	Type
54	A	1685	C
54	A	1686	A
54	A	1689	C
54	A	1690	C
54	A	1691	C
54	A	1699	C
54	A	1700	U
54	A	1701	U
54	A	1703	C
54	A	1704	U
54	A	1708	A
54	A	1713	A
54	A	1714	C
54	A	1715	C
54	A	1724	A
54	A	1727	A
54	A	1728	U
54	A	1748	G
54	A	1750	G
54	A	1751	A
54	A	1760	G
54	A	1768	G
54	A	1769	C
54	A	1770	G
54	A	1773	A
54	A	1777	A
54	A	1780	U
54	A	1791	G
54	A	1794	A
54	A	1797	G
54	A	1803	A
54	A	1804	A
54	A	1805	A
54	A	1812	C
54	A	1813	C
54	A	1817	C
54	A	1821	A
54	A	1823	A
54	A	1824	U
54	A	1827	C
54	A	1828	A
54	A	1829	A

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Mol	Chain	Res	Type
54	A	1832	A
54	A	1836	A
54	A	1839	C
54	A	1844	A
54	A	1849	C
54	A	1852	C
54	A	1854	U
54	A	1856	A
54	A	1867	A
54	A	1869	A
54	A	1870	A
54	A	1872	U
54	A	1878	U
54	A	1882	A
54	A	1883	G
54	A	1887	A
54	A	1888	G
54	A	1890	C
54	A	1892	A
54	A	1893	A
54	A	1901	C
54	A	1903	C
54	A	1905	C
54	A	1909	A
54	A	1918	G
54	A	1927	G
54	A	1939	G
54	A	1940	A
54	A	1944	C
54	A	1968	G
54	A	1972	A
54	A	1973	G
54	A	1974	A
54	A	1985	G
54	A	1987	G
54	A	1992	C
54	A	1993	A
54	A	1994	A
54	A	1995	A
54	A	1999	A
54	A	2000	C
54	A	2001	C

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Mol	Chain	Res	Type
54	A	2015	G
54	A	2021	U
54	A	2022	G
54	A	2029	A
54	A	2030	U
54	A	2031	A
54	A	2032	G
54	A	2033	A
54	A	2034	A
54	A	2036	C
54	A	2037	U
54	A	2039	A
54	A	2044	A
54	A	2053	U
54	A	2060	A
54	A	2065	A
54	A	2074	A
54	A	2079	C
54	A	2083	U
54	A	2085	A
54	A	2096	U
54	A	2097	A
54	A	2098	G
54	A	2105	G
54	A	2109	A
54	A	2110	A
54	A	2113	G
54	A	2124	A
54	A	2125	C
54	A	2126	U
54	A	2132	A
54	A	2136	C
54	A	2141	U
54	A	2142	A
54	A	2147	G
54	A	2154	A
54	A	2157	U
54	A	2159	U
54	A	2168	U
54	A	2171	U
54	A	2172	A
54	A	2173	G

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Mol	Chain	Res	Type
54	A	2174	G
54	A	2180	A
54	A	2181	A
54	A	2182	G
54	A	2183	C
54	A	2187	C
54	A	2193	U
54	A	2195	A
54	A	2197	G
54	A	2198	A
54	A	2199	A
54	A	2200	A
54	A	2207	A
54	A	2209	G
54	A	2210	C
54	A	2215	C
54	A	2217	C
54	A	2230	A
54	A	2233	U
54	A	2237	A
54	A	2239	A
54	A	2241	A
54	A	2242	U
54	A	2243	A
54	A	2244	U
54	A	2245	A
54	A	2246	A
54	A	2247	C
54	A	2257	C
54	A	2260	A
54	A	2262	C
54	A	2263	C
54	A	2269	G
54	A	2271	C
54	A	2280	C
54	A	2284	C
54	A	2287	U
54	A	2290	A
54	A	2291	A
54	A	2297	A
54	A	2299	U
54	A	2300	G

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Mol	Chain	Res	Type
54	A	2309	A
54	A	2315	A
54	A	2316	U
54	A	2322	C
54	A	2323	A
54	A	2324	U
54	A	2330	U
54	A	2332	C
54	A	2345	G
54	A	2371	U
54	A	2372	U
54	A	2374	A
54	A	2381	A
54	A	2386	C
54	A	2387	U
54	A	2388	A
54	A	2390	A
54	A	2393	C
54	A	2396	C
54	A	2397	C
54	A	2401	A
54	A	2405	C
54	A	2406	A
54	A	2407	U
54	A	2414	C
54	A	2415	C
54	A	2416	U
54	A	2417	C
54	A	2426	C
54	A	2427	C
54	A	2434	A
54	A	2435	G
54	A	2443	C
54	A	2444	A
54	A	2446	A
54	A	2451	A
54	A	2452	A
54	A	2457	A
54	A	2458	A
54	A	2464	G
54	A	2469	A
54	A	2471	G

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Mol	Chain	Res	Type
54	A	2478	G
54	A	2484	C
54	A	2488	C
54	A	2493	C
54	A	2500	A
54	A	2502	C
54	A	2506	A
54	A	2507	A
54	A	2508	C
54	A	2511	C
54	A	2512	A
54	A	2520	C
54	A	2521	A
54	A	2523	C
54	A	2526	C
54	A	2527	A
54	A	2530	A
54	A	2531	U
54	A	2536	G
54	A	2540	C
54	A	2544	C
54	A	2551	G
54	A	2552	U
54	A	2557	C
54	A	2558	A
54	A	2559	U
54	A	2563	U
54	A	2564	A
54	A	2570	C
54	A	2571	G
54	A	2575	U
54	A	2576	A
54	A	2577	C
54	A	2578	C
54	A	2579	C
54	A	2580	U
54	A	2581	A
54	A	2582	A
54	A	2583	C
54	A	2584	C
54	A	2586	U
54	A	2592	G

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Mol	Chain	Res	Type
54	A	2593	G
54	A	2594	U
54	A	2601	A
54	A	2603	C
54	A	2607	U
54	A	2618	U
54	A	2626	U
54	A	2627	G
54	A	2628	U
54	A	2629	A
54	A	2630	U
54	A	2632	A
54	A	2633	A
54	A	2634	U
54	A	2635	G
54	A	2640	C
54	A	2642	C
54	A	2644	A
54	A	2645	G
54	A	2647	G
54	A	2654	U
54	A	2655	G
54	A	2656	U
54	A	2660	U
54	A	2683	C
54	A	2684	C
54	A	2686	G
54	A	2693	A
54	A	2694	A
54	A	2695	G
54	A	2696	A
54	A	2697	G
54	A	2698	G
54	A	2706	A
54	A	2708	C
54	A	2709	A
54	A	2718	C
54	A	2719	G
54	A	2723	A
54	A	2724	G
54	A	2725	A
54	A	2732	G

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Mol	Chain	Res	Type
54	A	2733	G
54	A	2740	A
54	A	2743	U
54	A	2744	U
54	A	2745	A
54	A	2747	U
54	A	2749	A
54	A	2752	C
54	A	2754	A
54	A	2755	A
54	A	2756	C
54	A	2801	A
54	A	2804	A
54	A	2810	G
54	A	2814	G
54	A	2831	G
54	A	2832	A
54	A	2833	A
54	A	2844	G
54	A	2847	C
54	A	2851	A
54	A	2852	C
54	A	2854	U
54	A	2860	G
54	A	2861	A
54	A	2864	U
54	A	2865	C
54	A	2871	U
54	A	2880	A
54	A	2891	C
54	A	2896	G
54	A	2901	A
54	A	2906	C
54	A	2910	A
54	A	2911	C
54	A	2913	A
54	A	2917	G
54	A	2918	A
54	A	2919	A
54	A	2922	A
54	A	2926	A
54	A	2928	C

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Mol	Chain	Res	Type
54	A	2932	G
54	A	2935	A
54	A	2952	U
54	A	2955	U
54	A	2956	A
54	A	2958	A
54	A	2963	A
54	A	2965	A
54	A	2977	G
54	A	2978	U
54	A	2985	C
54	A	2989	G
54	A	2990	A
54	A	2991	U
54	A	2992	G
54	A	2993	U
54	A	2994	U
54	A	3000	A
54	A	3005	A
54	A	3012	U
54	A	3016	G
54	A	3022	G
54	A	3030	A
54	A	3041	U
54	A	3042	U
54	A	3049	U
54	A	3051	A
54	A	3053	A
54	A	3054	G
54	A	3056	C
54	A	3060	C
54	A	3063	G
54	A	3069	A
54	A	3072	U
54	A	3077	C
54	A	3084	A
54	A	3086	U
54	A	3089	A
54	A	3090	G
54	A	3092	U
54	A	3093	C
54	A	3096	U

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Mol	Chain	Res	Type
54	A	3098	U
54	A	3099	C
54	A	3100	U
54	A	3102	U
54	A	3108	U
54	A	3109	U
54	A	3114	U
54	A	3122	U
54	A	3123	G
54	A	3129	A
54	A	3131	G
54	A	3135	A
54	A	3141	A
54	A	3150	U
54	A	3151	A
54	A	3155	C
54	A	3157	C
54	A	3158	A
54	A	3160	A
54	A	3162	C
54	A	3168	C
54	A	3169	C
54	A	3172	C
54	A	3173	G
54	A	3180	A
54	A	3182	A
54	A	3189	C
54	A	3190	A
54	A	3196	G
54	A	3202	U
54	A	3206	C
54	A	3207	A
54	A	3213	A
54	A	3217	A
54	A	3218	A
54	A	3220	A
55	B	1607	U
55	B	1608	G
55	B	1609	U
55	B	1611	G
55	B	1614	U
55	B	1615	A

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Mol	Chain	Res	Type
55	B	1622	A
55	B	1625	A
55	B	1628	C
55	B	1631	C
55	B	1632	U
55	B	1633	U
55	B	1634	A
55	B	1641	G
55	B	1643	A
55	B	1644	G
55	B	1645	A
55	B	1646	U
55	B	1650	A
55	B	1651	A
55	B	1661	A
55	B	1667	C
55	B	1669	G
56	24	2	U
56	24	3	U
56	24	4	A
56	24	7	G
56	24	9	A
56	24	10	G
56	24	13	U
56	24	14	A
56	24	16	A
56	24	17	U
56	24	18	U
56	24	19	A
56	24	20	U
56	24	21	C
56	24	22	A
56	24	27	A
56	24	31	C
56	24	36	A
56	24	40	U
56	24	41	G
56	24	45	A
56	24	46	G
56	24	48	U
56	24	50	A
56	24	51	G

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Mol	Chain	Res	Type
56	24	52	C
56	24	54	U
56	24	55	C
56	24	56	A
56	24	57	C
56	24	58	A
56	24	59	G
56	24	60	C
56	24	62	C
56	24	63	C
56	24	64	A
56	24	68	A

All (24) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
54	A	1703	C
54	A	1811	A
54	A	1823	A
54	A	1871	A
54	A	2021	U
54	A	2030	U
54	A	2125	C
54	A	2182	G
54	A	2186	C
54	A	2243	A
54	A	2245	A
54	A	2457	A
54	A	2507	A
54	A	2530	A
54	A	2606	U
54	A	2653	C
54	A	2905	A
54	A	2910	A
54	A	2989	G
54	A	3041	U
54	A	3092	U
54	A	3113	A
55	B	1607	U
56	24	1	G

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

1 non-standard protein/DNA/RNA residue is 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
58	MEQ	C	73	58	8,9,10	0.98	1 (12%)	5,10,12	0.72	0

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
58	MEQ	C	73	58	-	4/8/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	C	73	MEQ	CE-NE2	-2.03	1.42	1.45

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	C	73	MEQ	C-CA-CB-CG
58	C	73	MEQ	CG-CD-NE2-CE
58	C	73	MEQ	OE1-CD-NE2-CE
58	C	73	MEQ	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 95 ligands modelled in this entry, 94 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
62	PNS	v	101	53	14,20,21	2.22	4 (28%)	18,26,29	1.87	5 (27%)

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
62	PNS	v	101	53	-	9/24/26/27	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	v	101	PNS	C39-N41	5.17	1.45	1.33
62	v	101	PNS	C34-N36	5.00	1.45	1.33
62	v	101	PNS	O40-C39	-2.86	1.17	1.23
62	v	101	PNS	O35-C34	-2.24	1.19	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	v	101	PNS	C37-N36-C34	-4.01	115.34	122.55
62	v	101	PNS	C31-C29-C32	3.34	114.47	108.77
62	v	101	PNS	C38-C39-N41	3.34	122.42	116.34
62	v	101	PNS	C32-C34-N36	2.47	121.16	116.48
62	v	101	PNS	O40-C39-C38	-2.10	118.21	122.02

There are no chirality outliers.

All (9) torsion outliers are listed below:

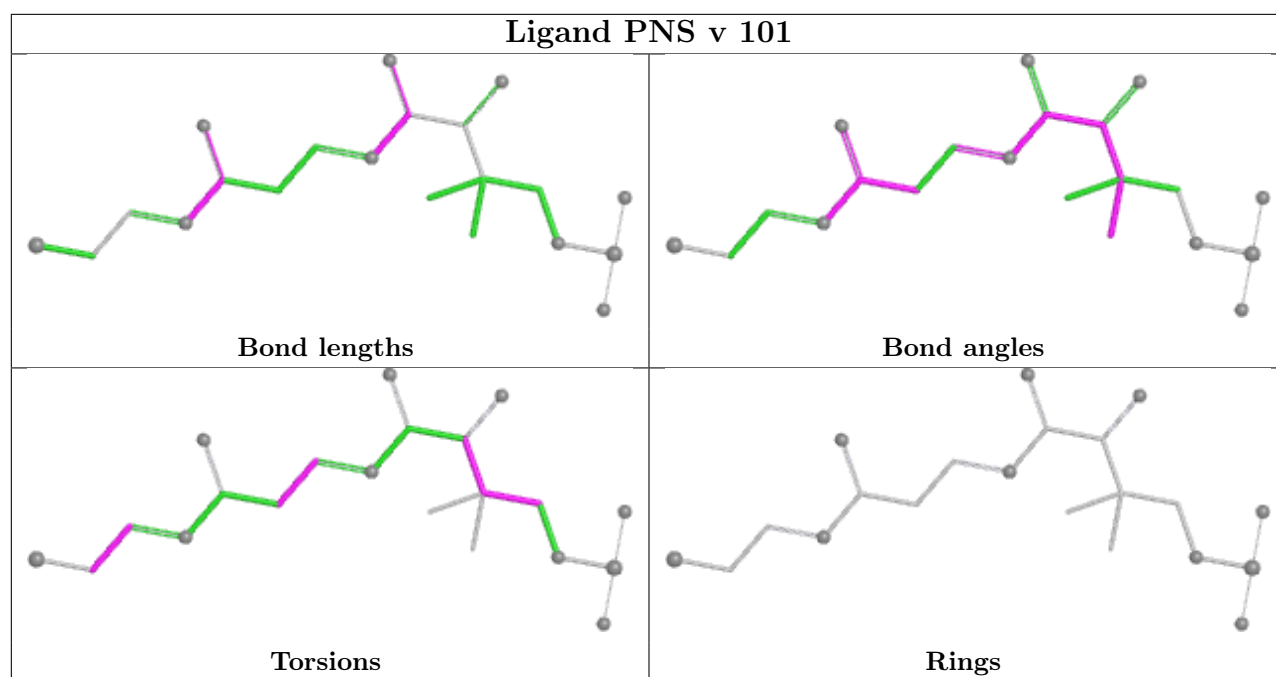
Mol	Chain	Res	Type	Atoms
62	v	101	PNS	C28-C29-C32-O33
62	v	101	PNS	C28-C29-C32-C34
62	v	101	PNS	C30-C29-C32-O33
62	v	101	PNS	C30-C29-C32-C34
62	v	101	PNS	C31-C29-C32-O33
62	v	101	PNS	C31-C29-C32-C34
62	v	101	PNS	N41-C42-C43-S44
62	v	101	PNS	N36-C37-C38-C39
62	v	101	PNS	O27-C28-C29-C30

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
62	v	101	PNS	4	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
17	U	1
28	6	1
16	T	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	U	124:ASP	C	125:ASP	N	3.71
1	6	28:ARG	C	29:THR	N	1.18
1	T	58:VAL	C	59:TYR	N	1.14

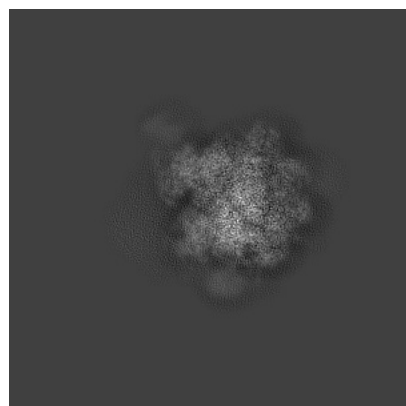
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11643. These allow visual inspection of the internal detail of the map and identification of artifacts.

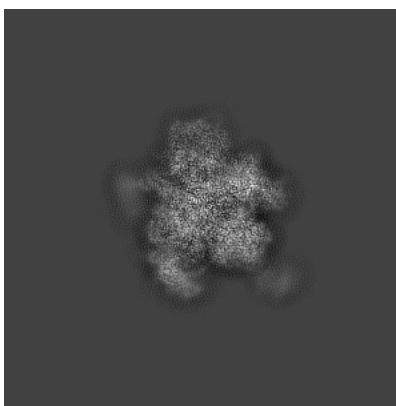
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

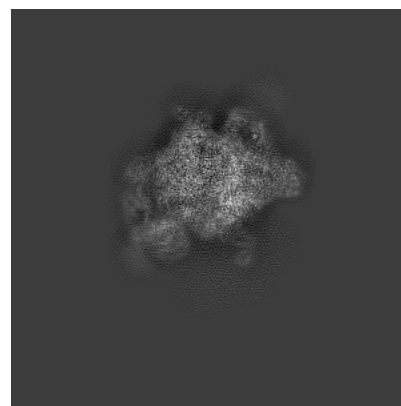
6.1.1 Primary map



X

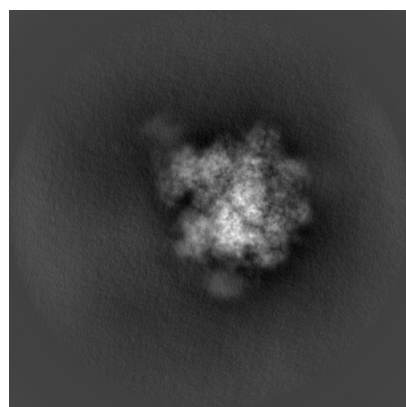


Y

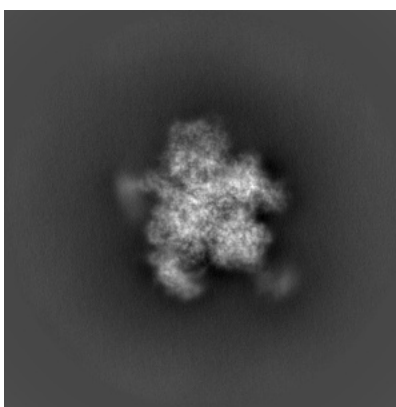


Z

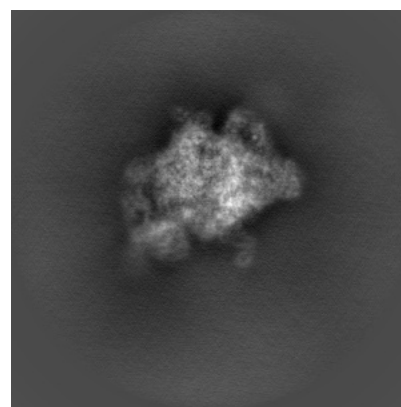
6.1.2 Raw map



X



Y

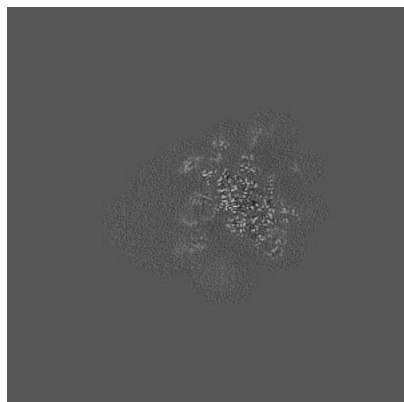


Z

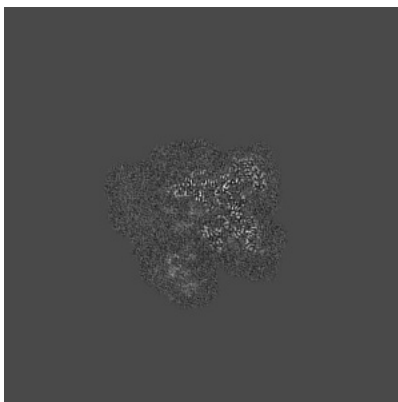
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

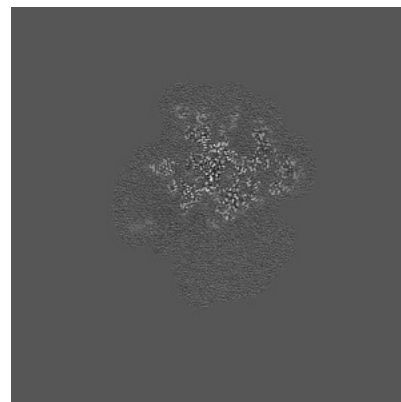
6.2.1 Primary map



X Index: 256

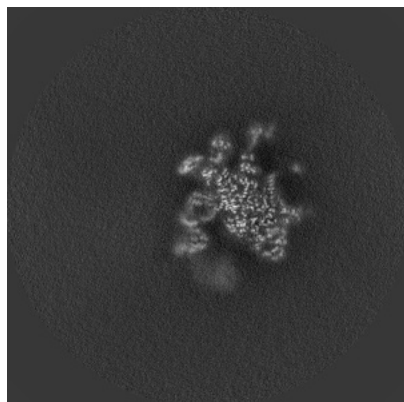


Y Index: 256

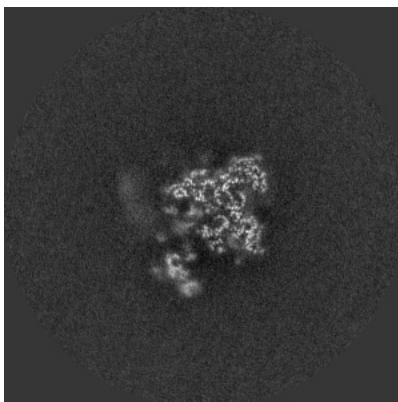


Z Index: 256

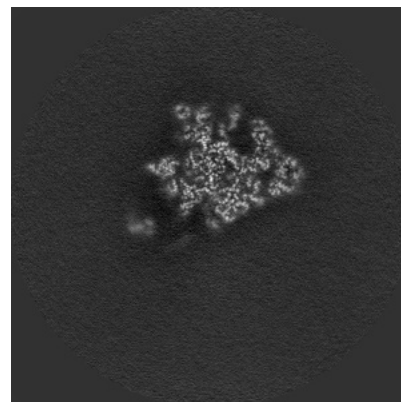
6.2.2 Raw map



X Index: 256



Y Index: 256

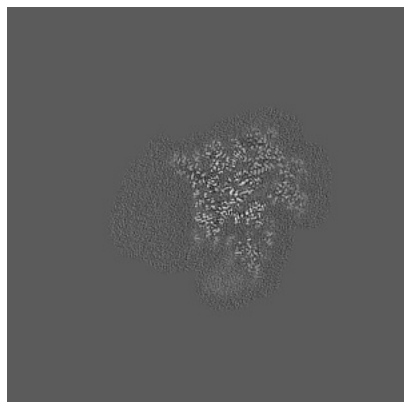


Z Index: 256

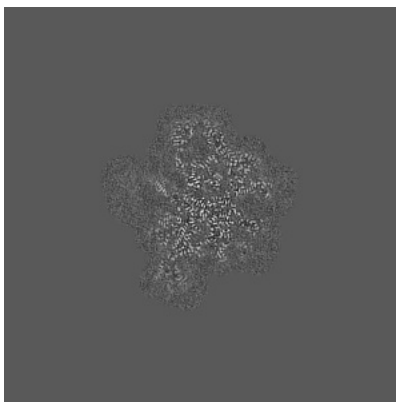
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

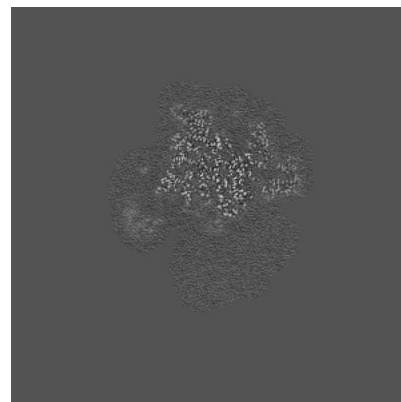
6.3.1 Primary map



X Index: 284

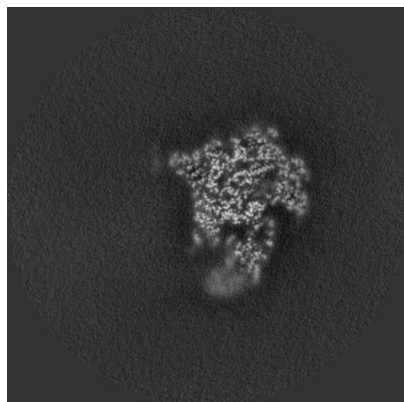


Y Index: 293

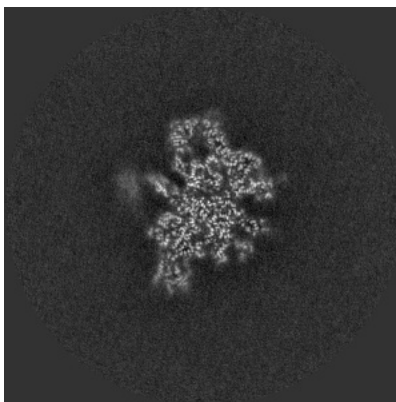


Z Index: 246

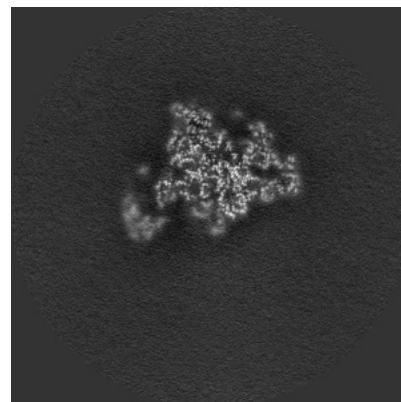
6.3.2 Raw map



X Index: 285



Y Index: 293

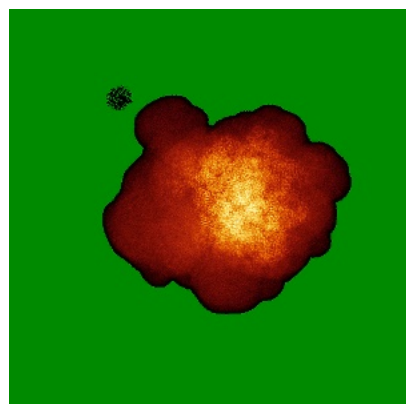


Z Index: 243

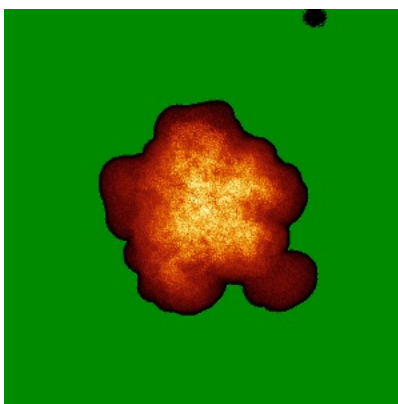
The images above show the largest variance slices of the map in three orthogonal directions.

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

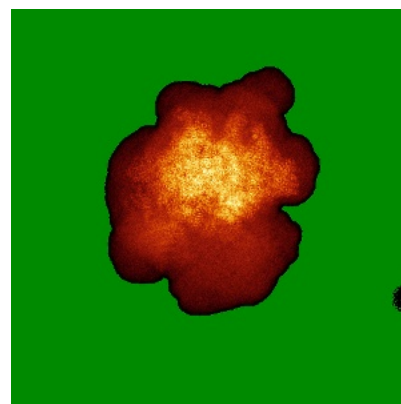
6.4.1 Primary map



X

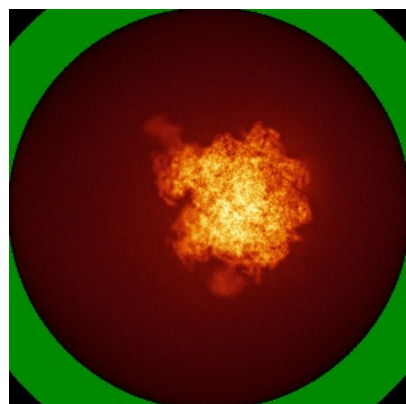


Y

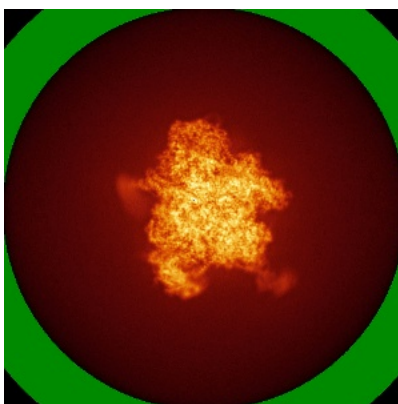


Z

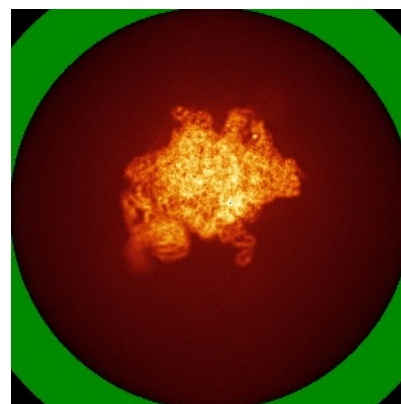
6.4.2 Raw map



X



Y

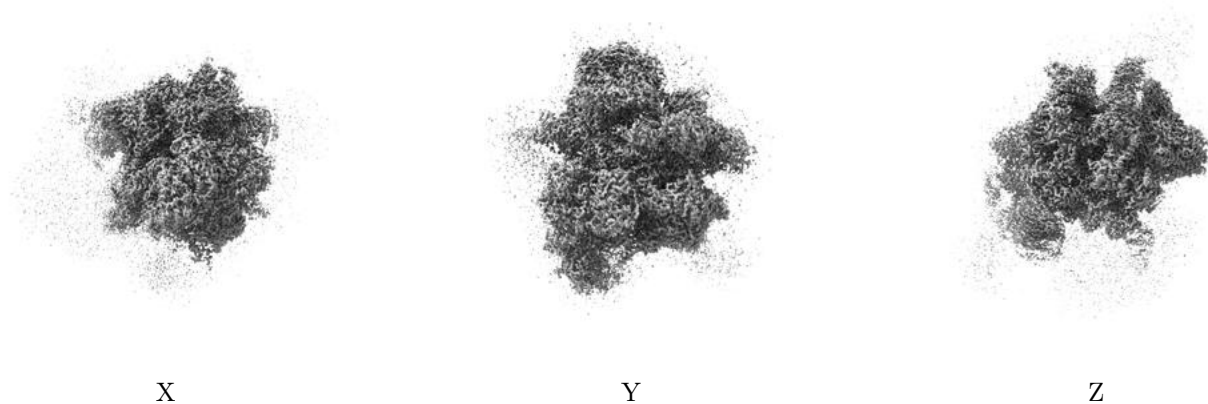


Z

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

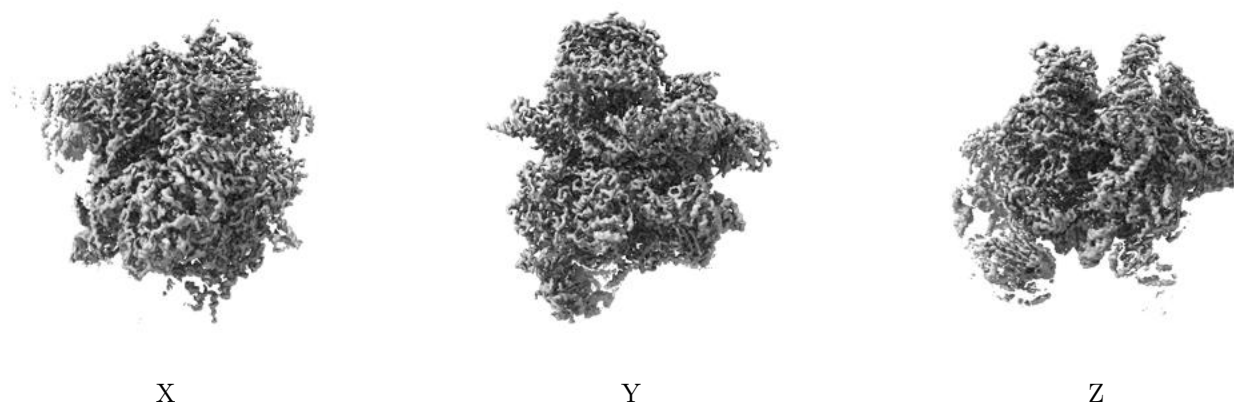
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.11. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

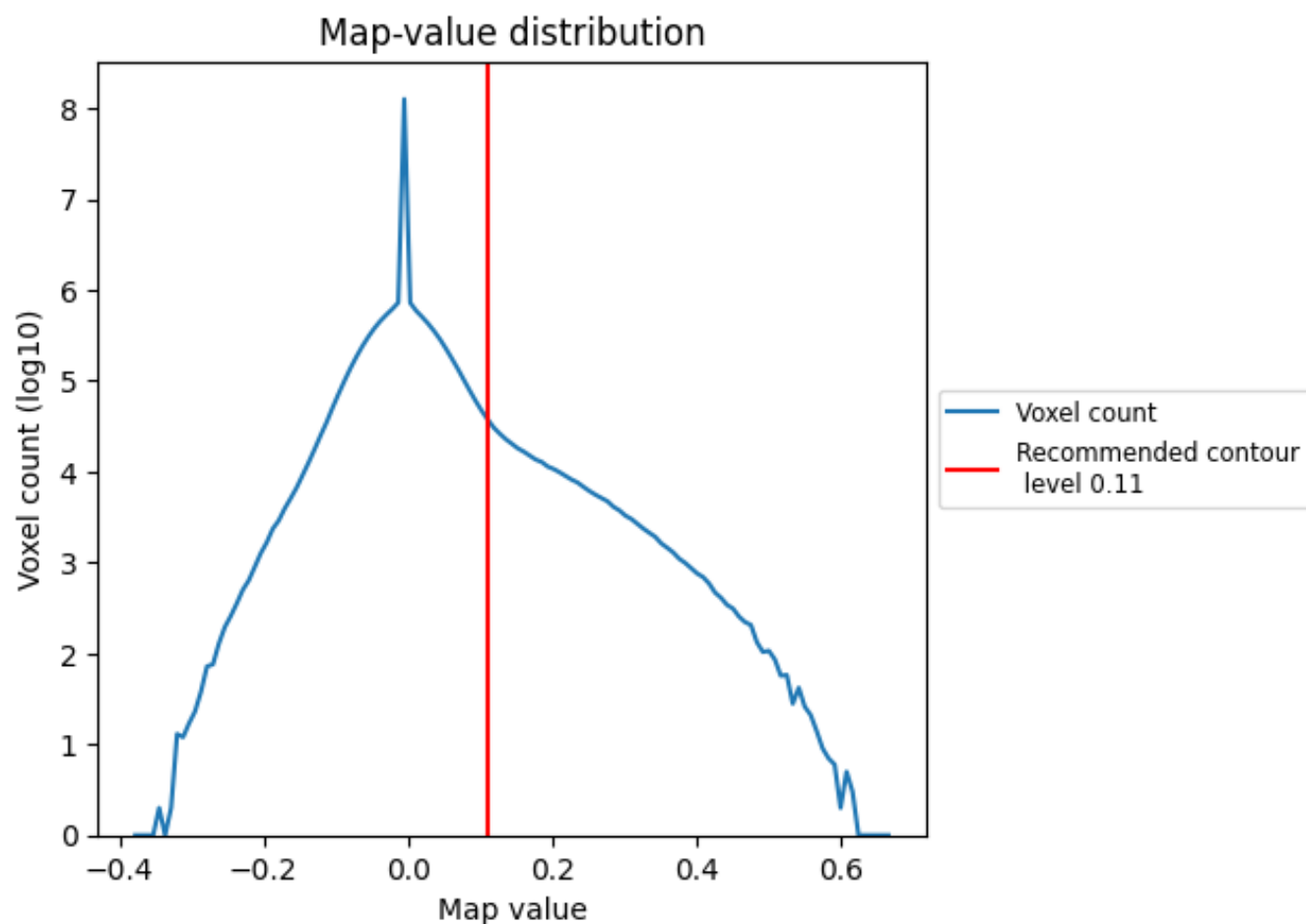
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

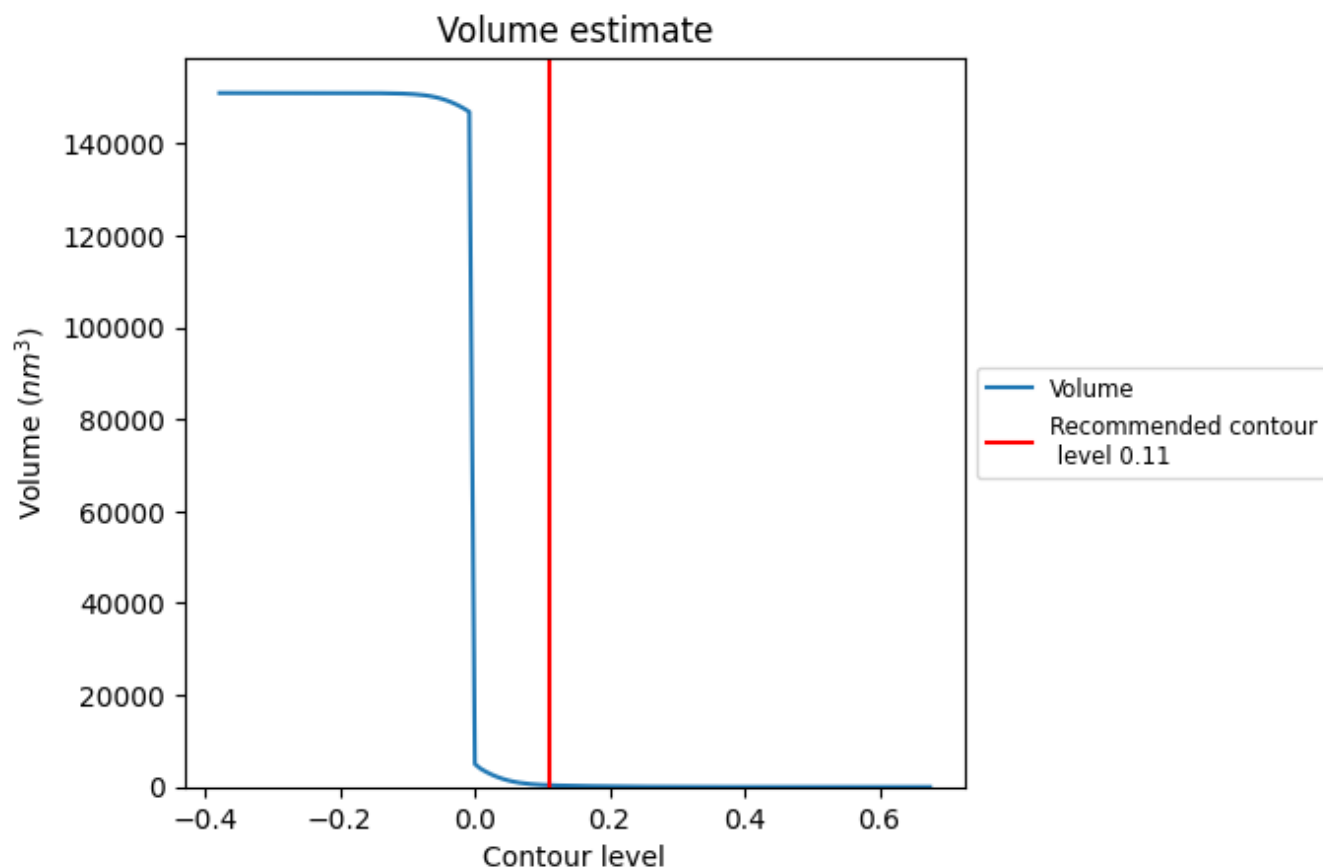
This section contains the results of statistical analysis of the map.

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.

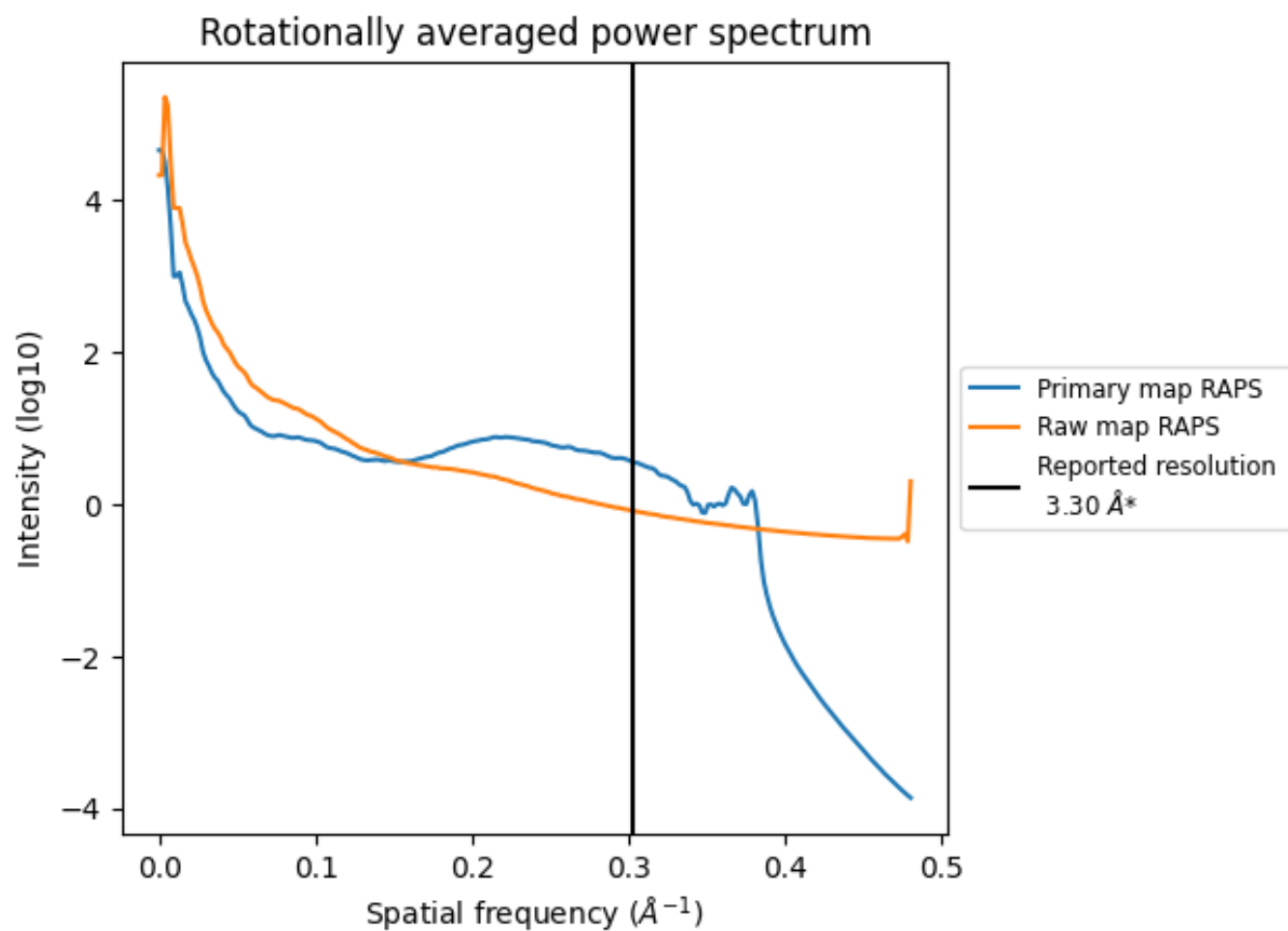
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 383 nm^3 ; this corresponds to an approximate mass of 346 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 ⓘ

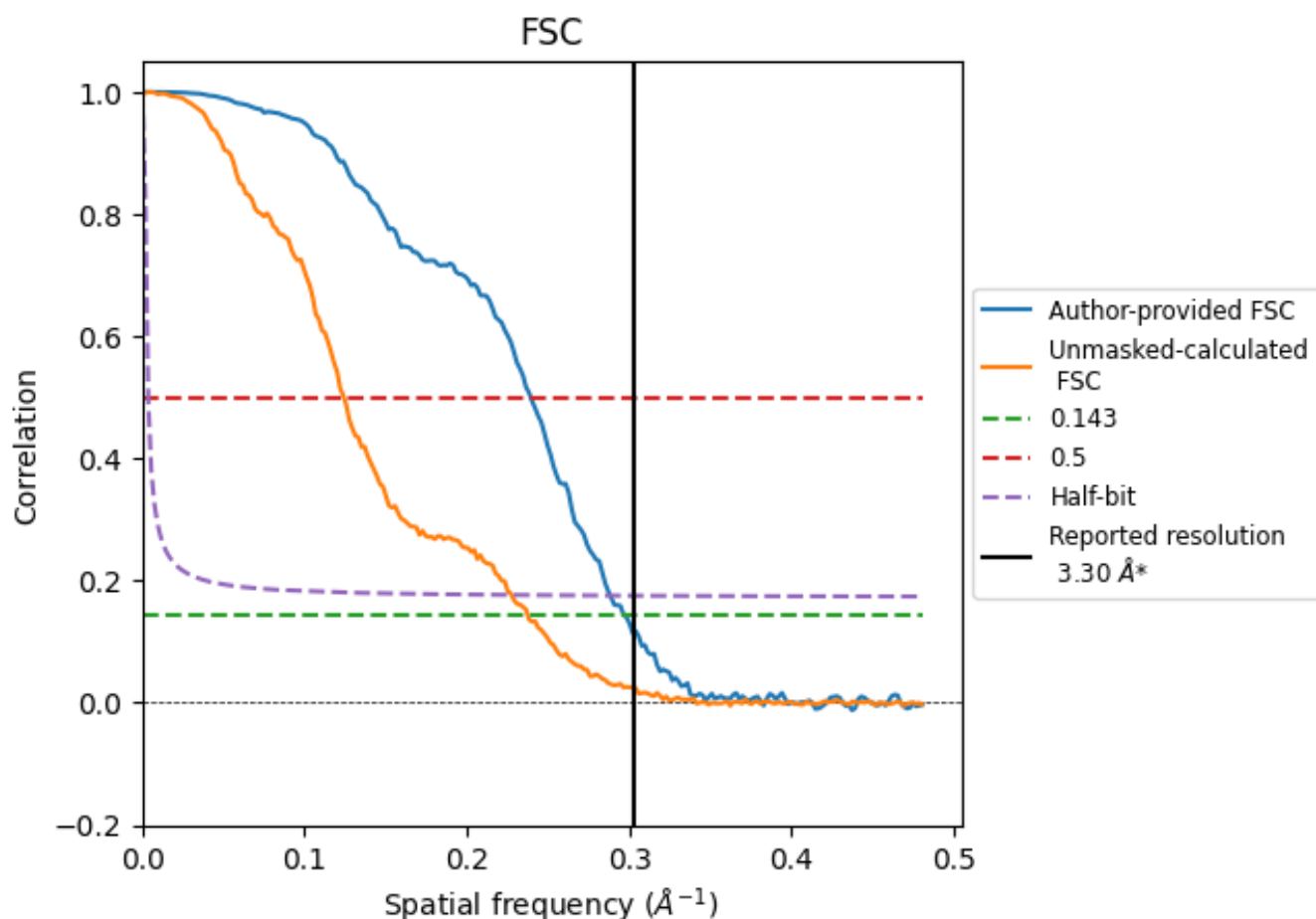


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.303 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.36	4.18	3.47
Unmasked-calculated*	4.21	8.05	4.39

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.21 differs from the reported value 3.3 by more than 10 %

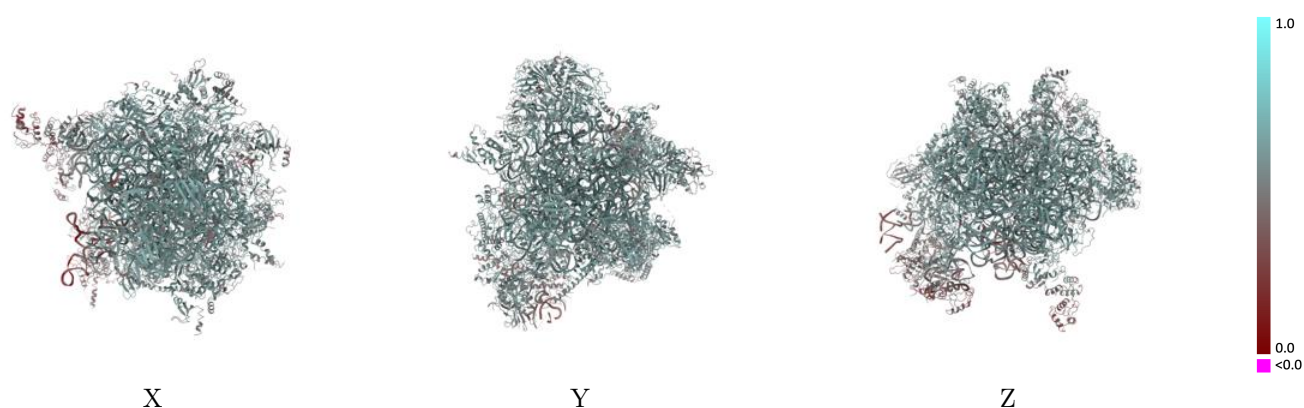
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11643 and PDB model 7A5H. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)

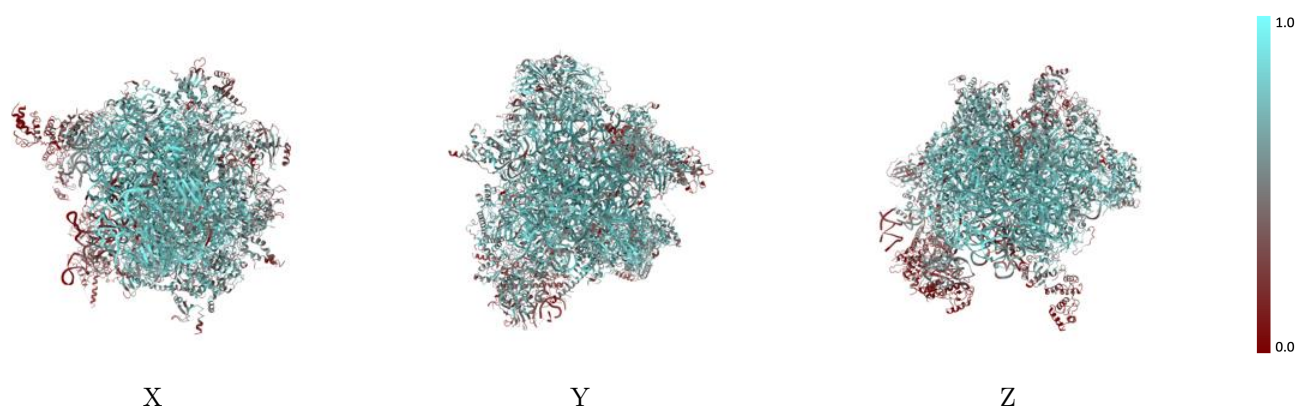
This section was not generated.

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



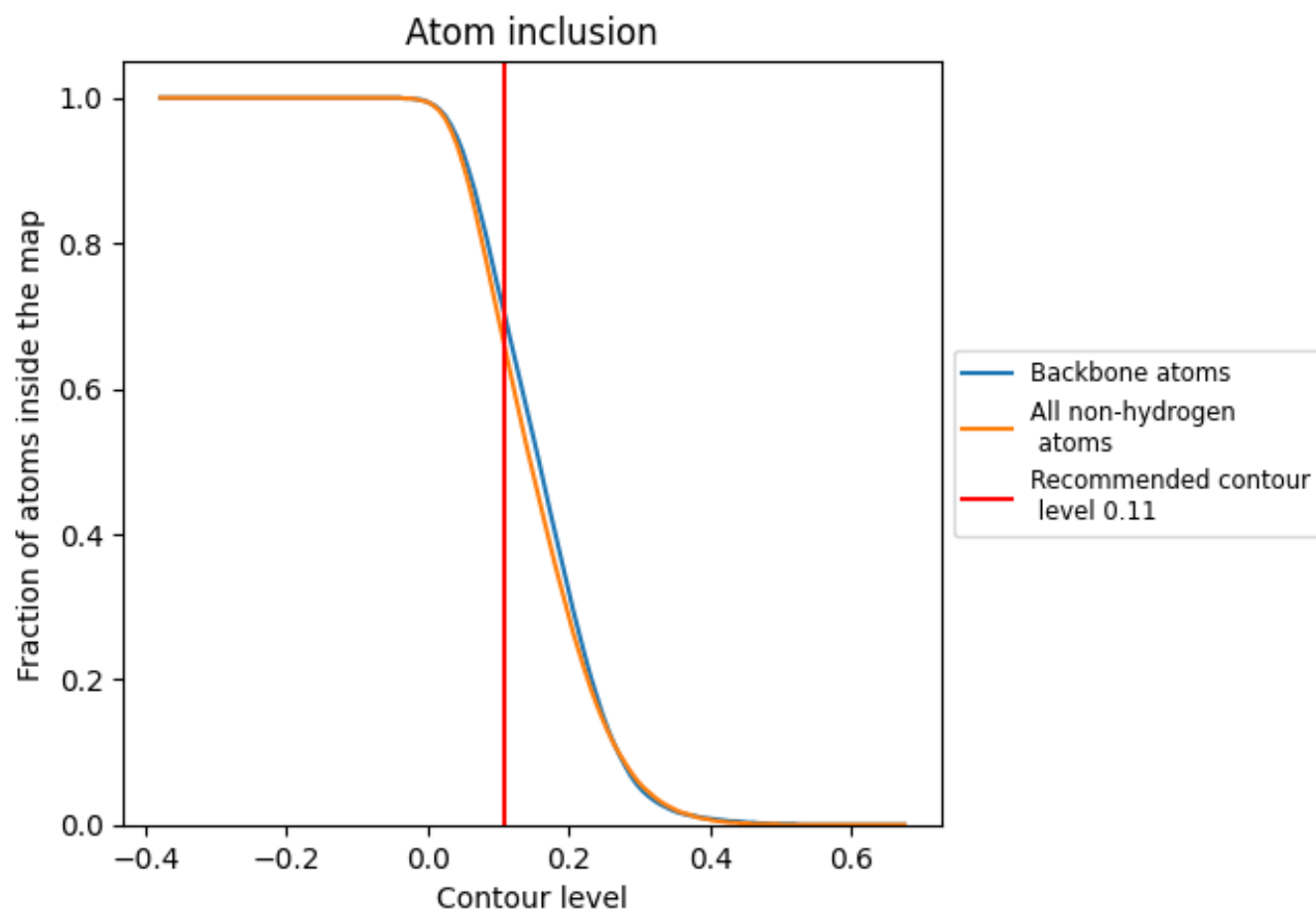
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.11).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 65% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6530	0.5530
0	0.6350	0.5740
1	0.6480	0.5620
2	0.8260	0.6210
24	0.1940	0.2980
3	0.7890	0.6150
5	0.6450	0.5580
6	0.5390	0.5260
7	0.5050	0.5290
8	0.1420	0.3890
9	0.6120	0.5630
A	0.8360	0.5920
B	0.3870	0.3880
C	0.3120	0.5120
D	0.7190	0.5840
E	0.7120	0.5830
F	0.7100	0.5860
G	0.3440	0.4660
H	0.5320	0.5450
I	0.3490	0.4630
J	0.1800	0.3930
K	0.7510	0.5950
L	0.6890	0.5770
M	0.7260	0.5850
N	0.6970	0.5850
O	0.7350	0.5850
P	0.6260	0.5610
Q	0.6390	0.5660
R	0.7600	0.6050
S	0.7230	0.5880
T	0.7110	0.5900
U	0.6160	0.5460
V	0.4920	0.5220
W	0.7480	0.6040
X	0.6310	0.5630



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Chain	Atom inclusion	Q-score
Y	 0.6850	 0.5840
Y2	 0.1080	 0.3260
Z	 0.7380	 0.5940
a	 0.6840	 0.5760
b	 0.7270	 0.5900
c	 0.6200	 0.5600
d	 0.4410	 0.5170
e	 0.0630	 0.3440
f	 0.2610	 0.4430
g	 0.6850	 0.5700
h	 0.4980	 0.5120
i	 0.7690	 0.6050
j	 0.6470	 0.5720
k	 0.3740	 0.4680
l	 0.5100	 0.5350
m	 0.1330	 0.3850
o	 0.7610	 0.6000
p	 0.5090	 0.5370
q	 0.4950	 0.5090
r	 0.7200	 0.5850
s	 0.6890	 0.5740
t	 0.1430	 0.3980
u	 0.4300	 0.5050
v	 0.2290	 0.4320
w	 0.0470	 0.3360