



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:21 PM UTC

PDB ID : 6SGA / pdb_00006sga
EMDB ID : EMD-10177
Title : Body domain of the mt-SSU assemblosome from Trypanosoma brucei
Authors : Saurer, M.; Ramrath, D.J.F.; Niemann, M.; Calderaro, S.; Prange, C.; Mattei, S.; Scaiola, A.; Leitner, A.; Bieri, P.; Horn, E.K.; Leibundgut, M.; Boehringer, D.; Schneider, A.; Ban, N.
Deposited on : 2019-08-03
Resolution : 3.10 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:

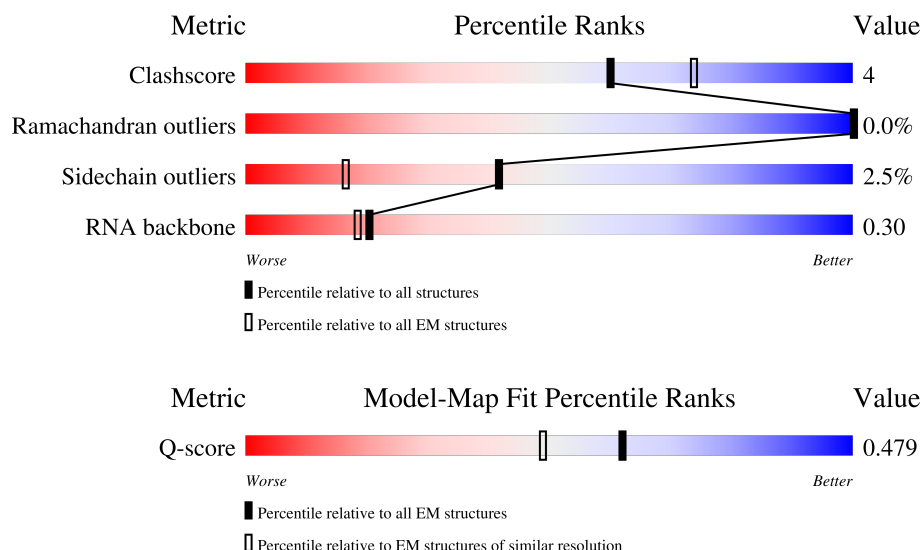
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

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

The reported resolution of this entry is 3.10 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.



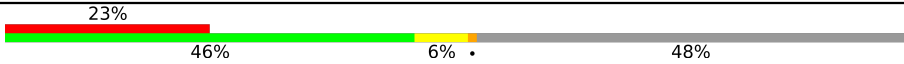
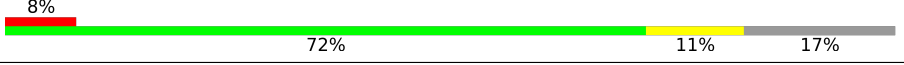
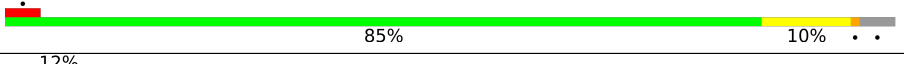
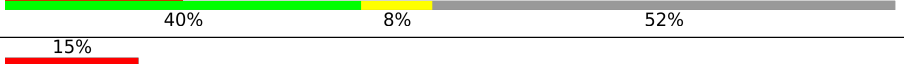
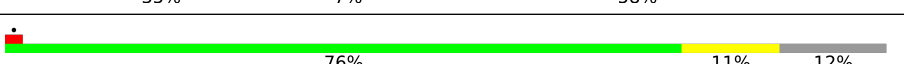
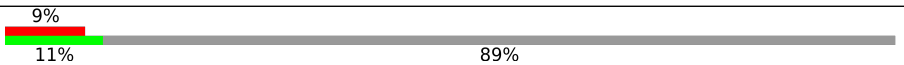
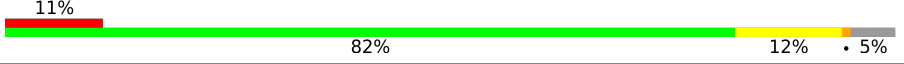
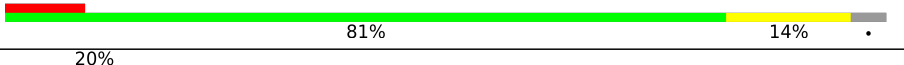
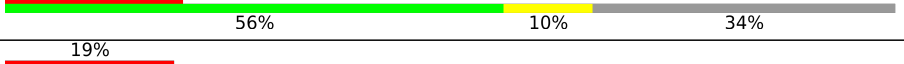
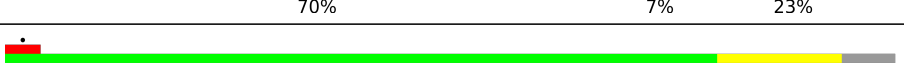
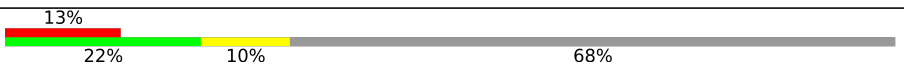
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	CE	435	20% 80% 10% 10%
2	CF	160	11% 83% 16% .
3	CH	282	10% 68% 11% 21%

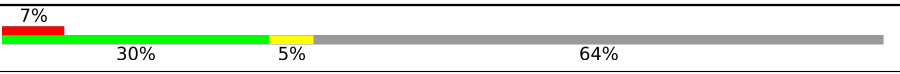
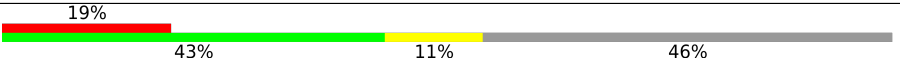
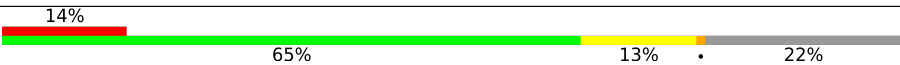
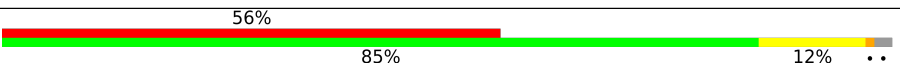
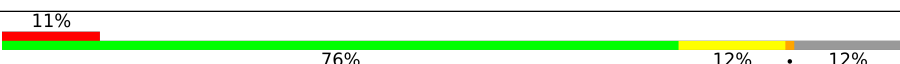
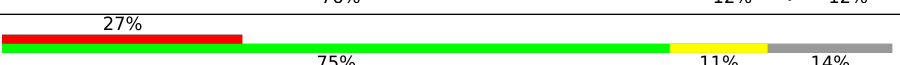
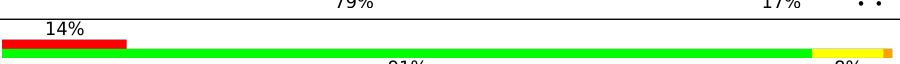
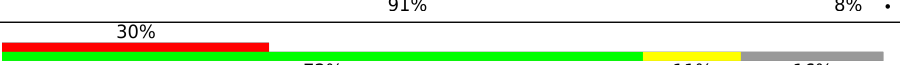
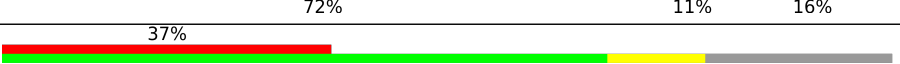
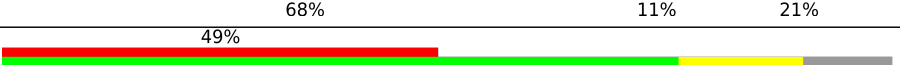
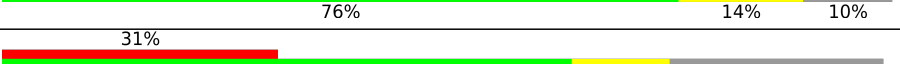
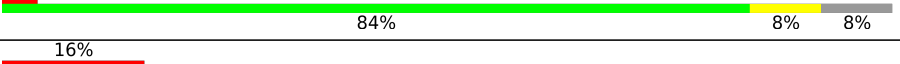
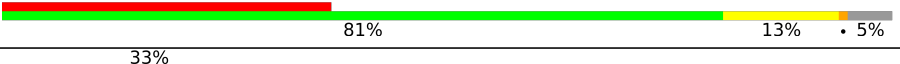
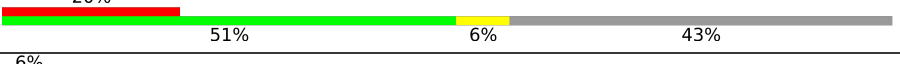
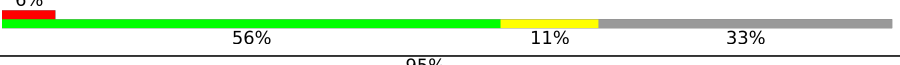
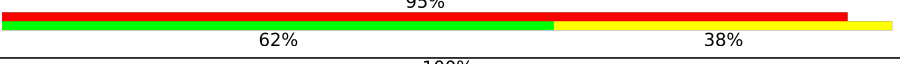
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Mol	Chain	Length	Quality of chain
4	CK	326	
5	CO	429	
6	CP	188	
7	CQ	336	
8	CR	320	
9	Ca	602	
10	Cb	311	
11	Cd	440	
12	Cj	257	
13	Cn	250	
14	Cp	187	
15	DD	812	
16	DI	407	
17	DL	307	
18	DO	282	
19	DP	274	
20	DR	270	
21	DU	228	
22	DZ	94	
23	F2	1024	
24	F3	966	
25	F5	754	
26	F6	676	
27	F7	679	
28	F8	726	

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Mol	Chain	Length	Quality of chain
29	F9	608	
30	FA	642	
31	FB	579	
31	FC	579	
32	FE	553	
33	FJ	362	
34	FM	370	
34	FN	370	
35	FO	334	
36	FP	349	
37	FQ	307	
37	FR	307	
37	FS	307	
37	FT	307	
37	FU	307	
38	FW	263	
39	FX	239	
40	FY	188	
41	FZ	178	
42	Fa	171	
43	Fb	151	
44	Fc	148	
45	Fd	143	
46	UA	21	
47	UB	27	

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Mol	Chain	Length	Quality of chain
48	UC	10	
49	UD	9	
49	UM	9	
49	UQ	9	
50	UE	45	
50	UP	45	
51	UF	11	
52	UG	17	
53	UH	5	
54	UI	8	
54	UN	8	
55	UJ	16	
56	UL	22	
57	UO	30	
58	UU	24	
59	UY	468	
60	CA	474	
61	F1	1041	
62	FF	474	

2 Entry composition [i](#)

There are 66 unique types of molecules in this entry. The entry contains 137038 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 uS5m.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	CE	392	Total	C	N	O	S	0	0
			3147	1992	579	561	15		

- Molecule 2 is a protein called bS6m.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	CF	159	Total	C	N	O	S	0	0
			1317	835	234	242	6		

- Molecule 3 is a protein called uS8m.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	CH	222	Total	C	N	O	S	0	0
			1824	1144	349	321	10		

- Molecule 4 is a protein called uS11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	CK	171	Total	C	N	O	S	0	0
			1384	875	251	249	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CK	3	ARG	GLN	conflict	UNP Q389T7

- Molecule 5 is a protein called uS15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	CO	358	Total	C	N	O	S	0	0
			2979	1891	557	514	17		

- Molecule 6 is a protein called bS16m.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	CP	180	Total	C	N	O	S	0	0
			1489	956	274	250	9		

- Molecule 7 is a protein called uS17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	CQ	219	Total	C	N	O	S	0	0
			1805	1151	340	306	8		

- Molecule 8 is a protein called bS18m.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	CR	153	Total	C	N	O	S	0	0
			1274	821	233	218	2		

- Molecule 9 is a protein called mS22.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Ca	512	Total	C	N	O	S	0	0
			4340	2778	770	771	21		

- Molecule 10 is a protein called mS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Cb	153	Total	C	N	O	S	0	0
			1274	819	232	217	6		

- Molecule 11 is a protein called mS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Cd	185	Total	C	N	O	S	0	0
			1616	1032	297	279	8		

- Molecule 12 is a protein called mS34.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Cj	226	Total	C	N	O	S	0	0
			1792	1138	310	340	4		

- Molecule 13 is a protein called mS38.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	Cn	27	Total	C	N	O	0	0
			234	155	44	35		

- Molecule 14 is a protein called mS41.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Cp	178	Total	C	N	O	S	0	0
			1506	952	272	277	5		

- Molecule 15 is a protein called mS51 (KRIPP1).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	DD	786	Total	C	N	O	S	0	0
			6488	4110	1168	1169	41		

- Molecule 16 is a protein called mS56.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	DI	390	Total	C	N	O	S	0	0
			3182	2020	554	594	14		

- Molecule 17 is a protein called mS59.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	DL	203	Total	C	N	O	S	0	0
			1656	1059	296	291	10		

- Molecule 18 is a protein called mS62 (KRIPP14).

Mol	Chain	Residues	Atoms					AltConf	Trace
18	DO	204	Total	C	N	O	S	0	0
			1648	1031	300	307	10		

- Molecule 19 is a protein called mS63 (KRIPP16).

Mol	Chain	Residues	Atoms					AltConf	Trace
19	DP	212	Total	C	N	O	S	0	0
			1800	1156	321	314	9		

- Molecule 20 is a protein called mS65.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	DR	254	Total	C	N	O	S	0	0
			2042	1313	373	346	10		

- Molecule 21 is a protein called mS68.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	DU	219	Total	C	N	O	S	0	0
			1738	1095	308	331	4		

- Molecule 22 is a protein called mS73.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	DZ	30	Total	C	N	O	S	0	0
			254	167	41	45	1		

- Molecule 23 is a protein called mt-SAF2 (KRIPP2).

Mol	Chain	Residues	Atoms					AltConf	Trace
23	F2	915	Total	C	N	O	S	0	0
			7274	4570	1281	1384	39		

- Molecule 24 is a protein called mt-SAF3.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	F3	888	Total	C	N	O	S	0	0
			6879	4302	1222	1303	52		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F3	44	THR	ALA	conflict	UNP Q38E61
F3	190	VAL	ILE	conflict	UNP Q38E61
F3	303	ALA	SER	conflict	UNP Q38E61
F3	418	ASP	ASN	conflict	UNP Q38E61

- Molecule 25 is a protein called mt-SAF5.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	F5	480	Total	C	N	O	S	0	0
			3474	2167	646	647	14		

- Molecule 26 is a protein called mt-SAF6.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	F6	456	Total	C	N	O	S	0	0
			3646	2311	635	686	14		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F6	285	ARG	HIS	conflict	UNP Q38FQ8
F6	291	ILE	THR	conflict	UNP Q38FQ8
F6	602	ALA	VAL	conflict	UNP Q38FQ8
F6	676	CYS	PHE	conflict	UNP Q38FQ8

- Molecule 27 is a protein called mt-SAF7 (KRIPP10).

Mol	Chain	Residues	Atoms					AltConf	Trace
27	F7	662	Total	C	N	O	S	0	0
			5225	3322	918	950	35		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F7	36	ILE	THR	conflict	UNP Q57UW6
F7	470	GLU	LYS	conflict	UNP Q57UW6
F7	474	VAL	ALA	conflict	UNP Q57UW6

- Molecule 28 is a protein called mt-SAF8.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	F8	513	Total	C	N	O	S	0	0
			3934	2493	721	701	19		

- Molecule 29 is a protein called mt-SAF9.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	F9	216	Total	C	N	O	S	0	0
			1755	1088	325	337	5		

- Molecule 30 is a protein called mt-SAF10.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	FA	579	Total	C	N	O	S	0	0
			4421	2801	785	813	22		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
FA	173	ALA	THR	conflict	UNP Q386U1
FA	352	TYR	HIS	conflict	UNP Q386U1

- Molecule 31 is a protein called mt-SAF11.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	FB	377	Total	C	N	O	S	0	0
			3055	1928	574	543	10		
31	FC	311	Total	C	N	O	S	0	0
			2572	1629	488	447	8		

- Molecule 32 is a protein called mt-SAF13.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	FE	434	Total	C	N	O	S	0	0
			3523	2268	611	626	18		

- Molecule 33 is a protein called mt-SAF18.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	FJ	353	Total	C	N	O	S	0	0
			2917	1843	550	516	8		

- Molecule 34 is a protein called mt-SAF21.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	FM	326	Total	C	N	O	S	0	0
			2449	1515	449	465	20		
34	FN	319	Total	C	N	O	S	0	0
			2392	1478	436	458	20		

- Molecule 35 is a protein called mt-SAF22 (KRIPP17).

Mol	Chain	Residues	Atoms					AltConf	Trace
35	FO	324	Total	C	N	O	S	0	0
			2671	1674	509	474	14		

- Molecule 36 is a protein called mt-SAF23.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	FP	348	Total	C	N	O	S	0	0
			2643	1682	464	487	10		

- Molecule 37 is a protein called mt-SAF24.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	FQ	257	Total	C	N	O	S	0	0
			2003	1265	358	373	7		
37	FR	243	Total	C	N	O	S	0	0
			1923	1217	344	355	7		
37	FS	277	Total	C	N	O	S	0	0
			2198	1389	397	404	8		
37	FT	233	Total	C	N	O	S	0	0
			1854	1177	331	339	7		
37	FU	270	Total	C	N	O	S	0	0
			2105	1331	380	386	8		

- Molecule 38 is a protein called mt-SAF26.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	FW	247	Total	C	N	O	S	0	0
			2034	1272	384	371	7		

- Molecule 39 is a protein called mt-SAF27.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	FX	220	Total	C	N	O	S	0	0
			1741	1093	318	316	14		

- Molecule 40 is a protein called mt-SAF28.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	FY	65	Total	C	N	O	0	0
			544	343	102	99		

- Molecule 41 is a protein called mt-SAF29.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	FZ	133	Total	C	N	O	S	0	0
			973	605	181	185	2		

- Molecule 42 is a protein called mt-SAF30.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Fa	163	Total	C	N	O	S	0	0
			1323	860	236	223	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Fa	73	ALA	VAL	conflict	UNP Q57VU7

- Molecule 43 is a protein called mt-SAF31.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Fb	129	Total	C	N	O	S	0	0
			1091	701	198	184	8		

- Molecule 44 is a protein called mt-SAF32.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Fc	84	Total	C	N	O	S	0	0
			669	427	106	135	1		

- Molecule 45 is a protein called mt-SAF33.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Fd	96	Total	C	N	O	S	0	0
			758	481	147	122	8		

- Molecule 46 is a protein called UNK-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	UA	21	Total	C	N	O	0	0
			126	84	21	21		

- Molecule 47 is a protein called UNK-B.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	UB	27	Total	C	N	O	0	0
			162	108	27	27		

- Molecule 48 is a protein called UNK-C.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	UC	10	Total	C	N	O	0	0
			60	40	10	10		

- Molecule 49 is a protein called UNK-D, UNK-M, UNK-Q.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	UD	9	Total	C	N	O	0	0
			54	36	9	9		
49	UM	9	Total	C	N	O	0	0
			54	36	9	9		
49	UQ	9	Total	C	N	O	0	0
			54	36	9	9		

- Molecule 50 is a protein called UNK-E, UNK-P.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	UE	45	Total	C	N	O	0	0
			270	180	45	45		
50	UP	45	Total	C	N	O	0	0
			270	180	45	45		

- Molecule 51 is a protein called UNK-F.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	UF	11	Total	C	N	O	0	0
			66	44	11	11		

- Molecule 52 is a protein called UNK-G.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	UG	17	Total	C	N	O	0	0
			102	68	17	17		

- Molecule 53 is a protein called UNK-H.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	UH	5	Total	C	N	O	0	0
			30	20	5	5		

- Molecule 54 is a protein called UNK-I, UNK-M.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	UI	8	Total	C	N	O	0	0
			48	32	8	8		
54	UN	8	Total	C	N	O	0	0
			48	32	8	8		

- Molecule 55 is a protein called UNK-J.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	UJ	16	Total	C	N	O	0	0
			96	64	16	16		

- Molecule 56 is a protein called UNK-L.

Mol	Chain	Residues	Atoms				AltConf	Trace
56	UL	22	Total	C	N	O	0	0
			132	88	22	22		

- Molecule 57 is a protein called UNK-O.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	UO	30	Total	C	N	O	0	0
			180	120	30	30		

- Molecule 58 is a protein called UNK-U.

Mol	Chain	Residues	Atoms				AltConf	Trace
58	UU	24	Total	C	N	O	0	0
			144	96	24	24		

- Molecule 59 is a protein called UNK-I.

Mol	Chain	Residues	Atoms				AltConf	Trace
59	UY	468	Total	C	N	O	0	0
			2808	1872	468	468		

- Molecule 60 is a RNA chain called 9S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	CA	463	Total	C	N	O	P	0	0
			8851	3940	1294	3153	464		

- Molecule 61 is a protein called mt-SAF1 (RSM22).

Mol	Chain	Residues	Atoms					AltConf	Trace
61	F1	56	Total	C	N	O	S	0	0
			465	281	107	76	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F1	707	SER	GLY	conflict	UNP Q385R2
F1	973	THR	MET	conflict	UNP Q385R2

- Molecule 62 is a protein called mt-SAF14.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	FF	16	Total	C	N	O	S	0	0
			141	89	30	20	2		

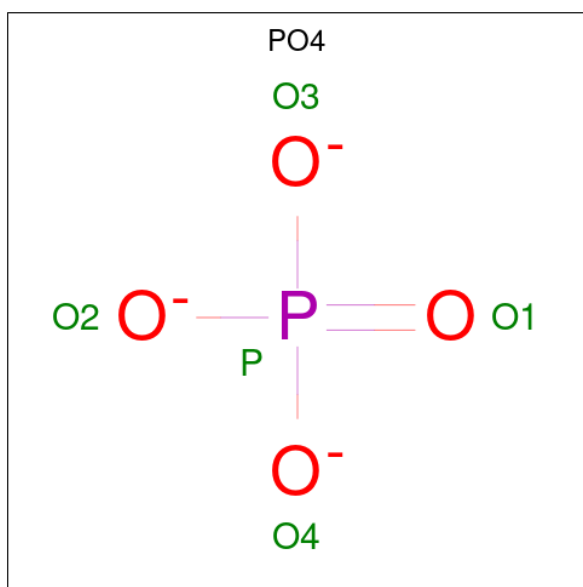
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
FF	70	ALA	PRO	conflict	UNP Q57W60
FF	179	PHE	LEU	conflict	UNP Q57W60

- Molecule 63 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

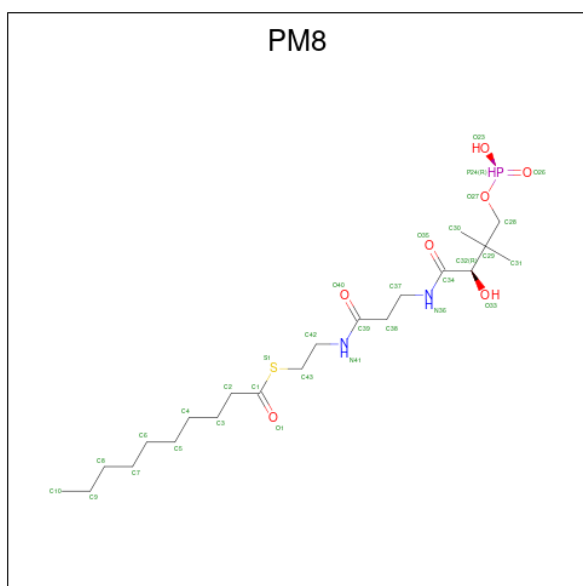
Mol	Chain	Residues	Atoms		AltConf
63	FPA	1	Total	Mg	0
			1	1	
63	FWB	1	Total	Mg	0
			1	1	
63	CAA	1	Total	Mg	0
			1	1	
63	CAB	1	Total	Mg	0
			1	1	

- Molecule 64 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			AltConf
64	FWA	1	Total	O	P	0
			5	4	1	

- Molecule 65 is S-(2-{[N-(2-HYDROXY-4-{[HYDROXY(OXIDO)PHOSPHINO]OXY}-3,3-DIMETHYLBUTANOYL)-BETA-ALANYL]AMINO}ETHYL) DECANETHIOATE (CCD ID: PM8) (formula: $C_{21}H_{41}N_2O_7PS$).



Mol	Chain	Residues	Atoms						AltConf
65	FcA	1	Total	C	N	O	P	S	0
			32	21	2	7	1	1	

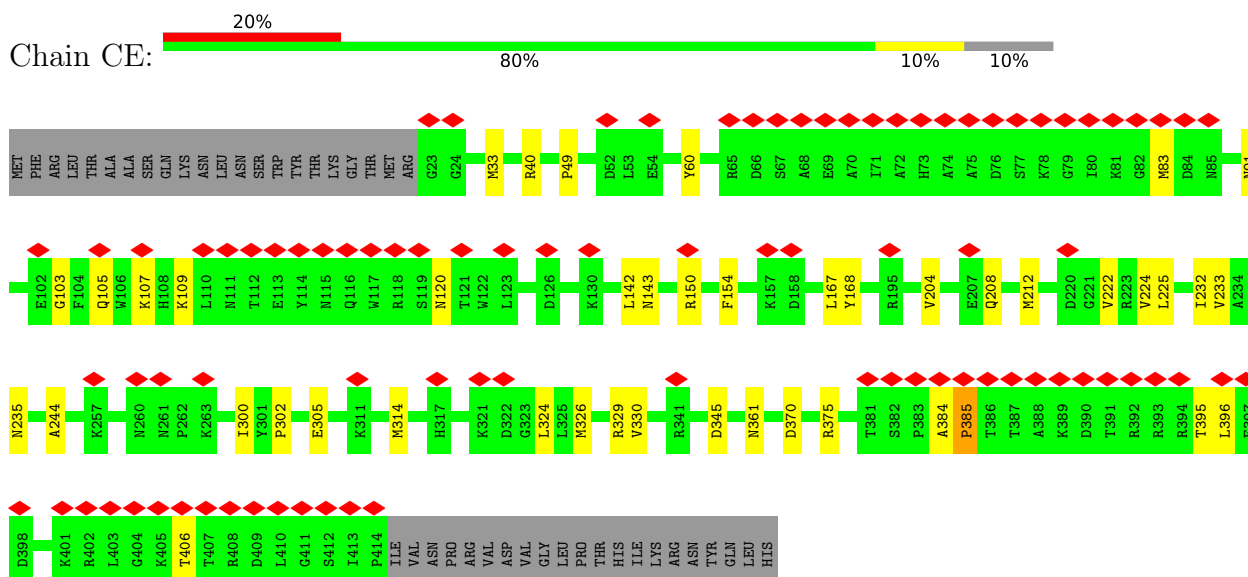
- Molecule 66 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
66	FdA	1	Total	Zn	0
			1	1	

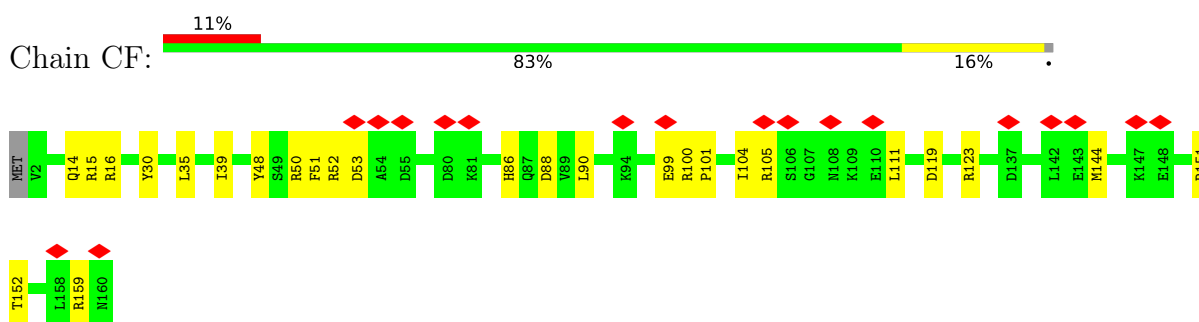
3 Residue-property plots [i](#)

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

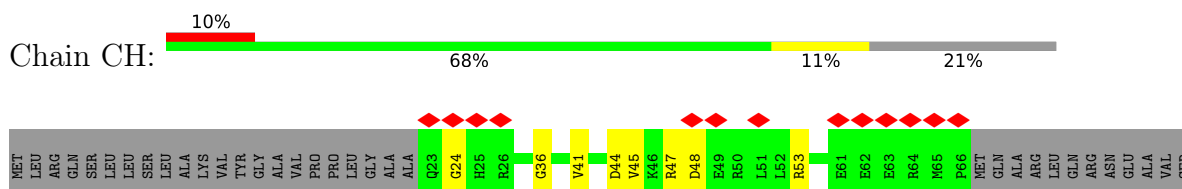
- Molecule 1: uS5m

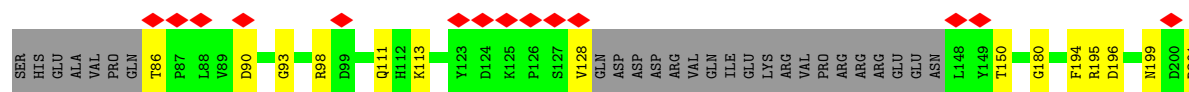


- Molecule 2: bS6m

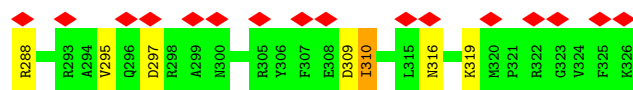
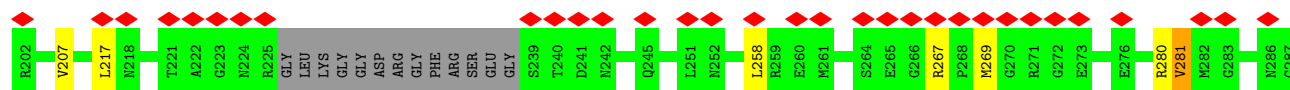
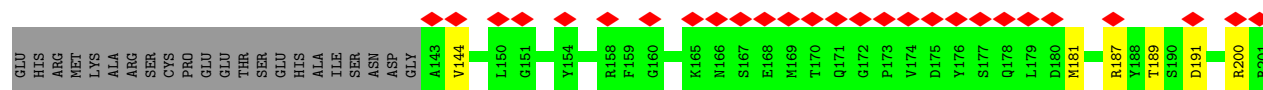
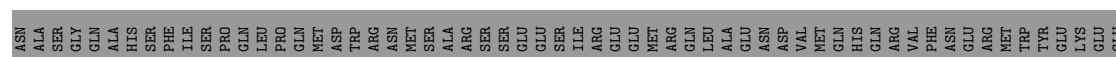
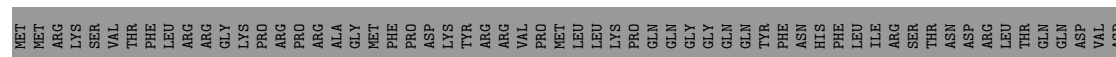


- Molecule 3: uS8m

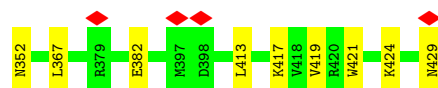
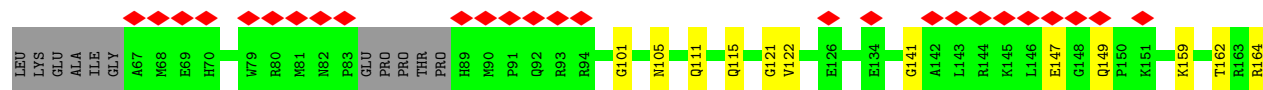
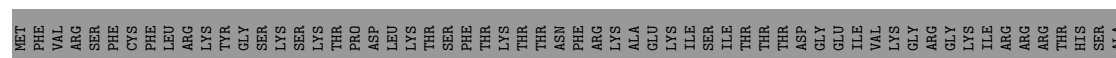
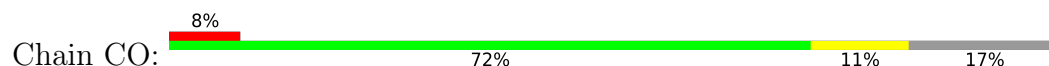




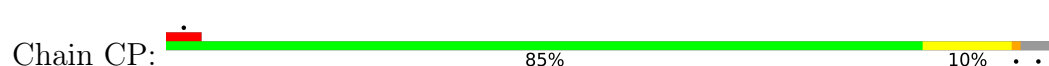
• Molecule 4: uS11m

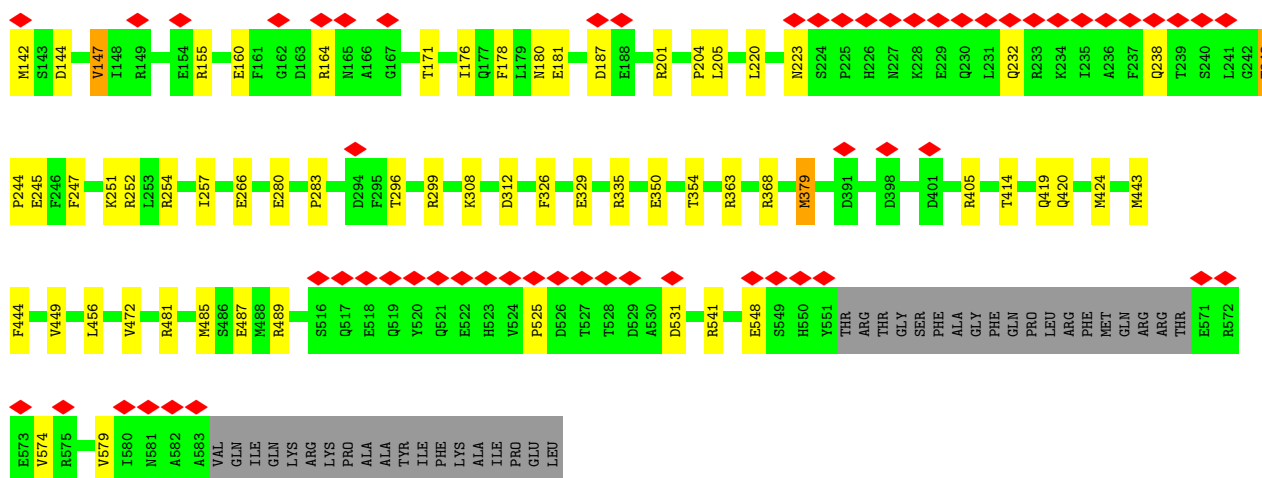


• Molecule 5: uS15m

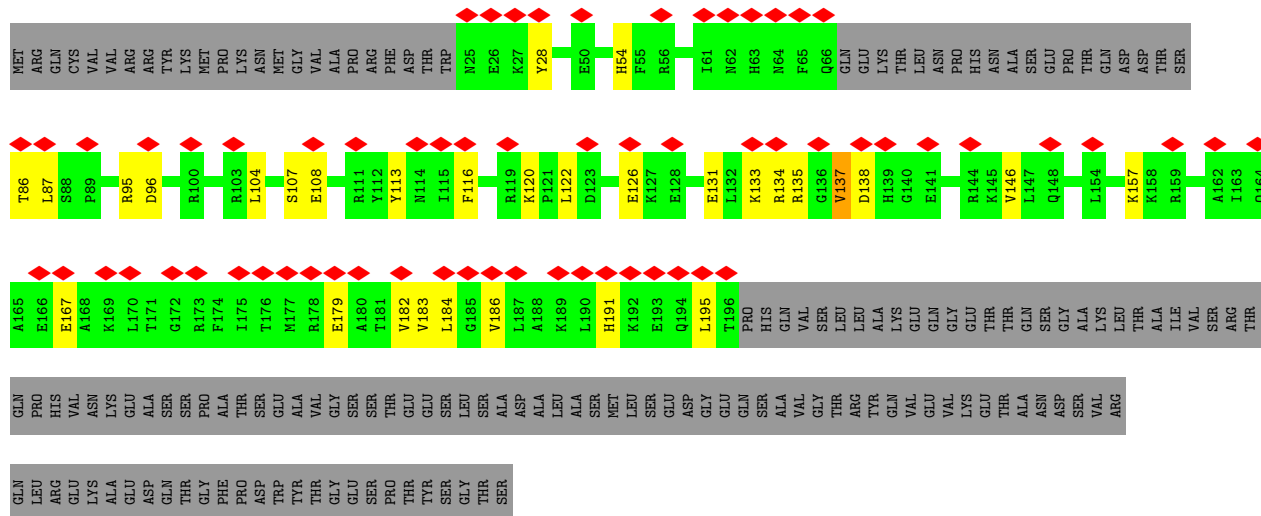
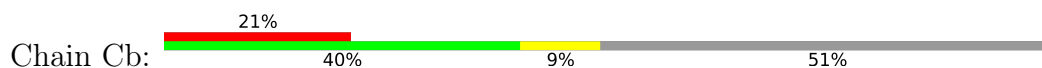


• Molecule 6: bS16m

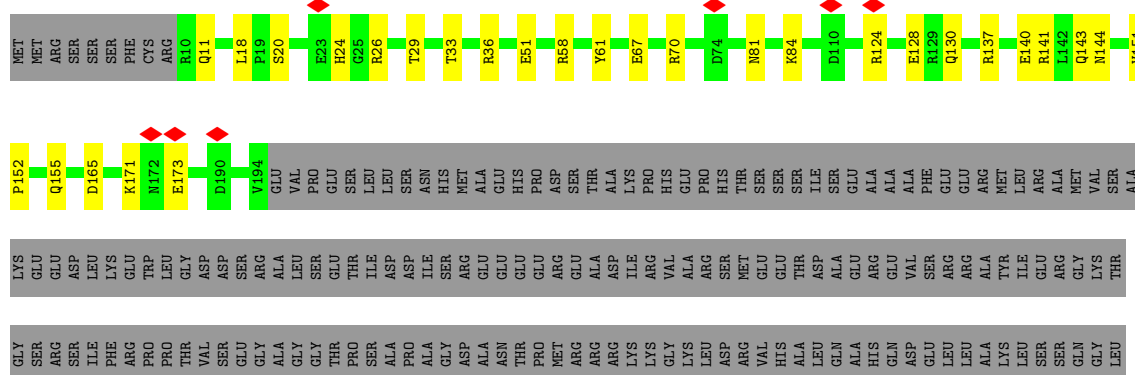
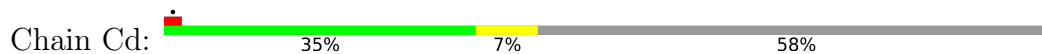




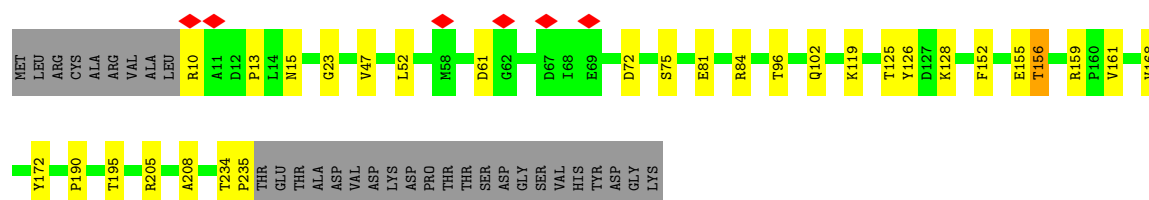
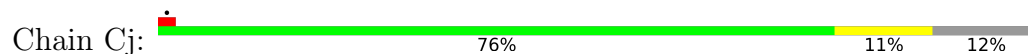
• Molecule 10: mS23



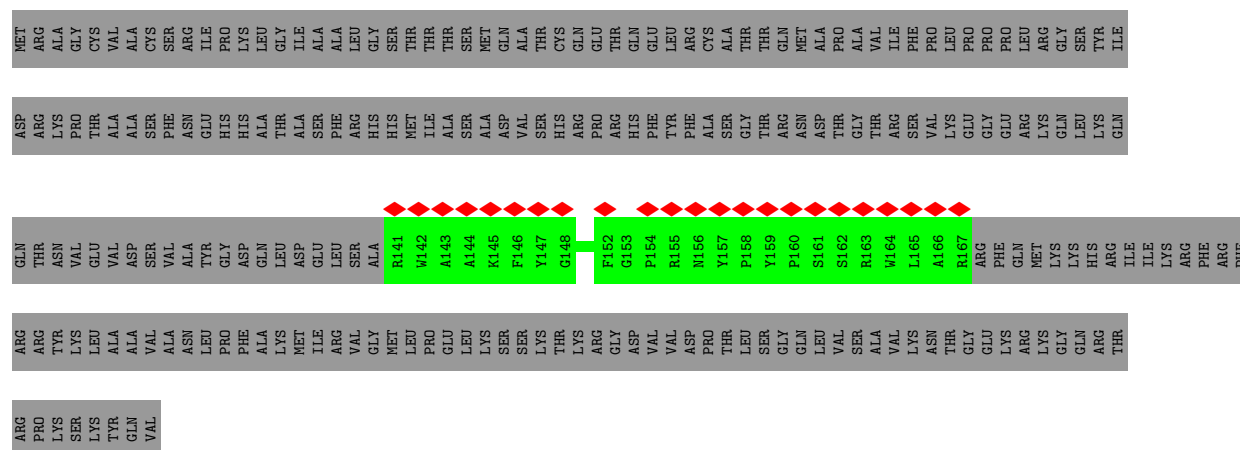
• Molecule 11: mS26



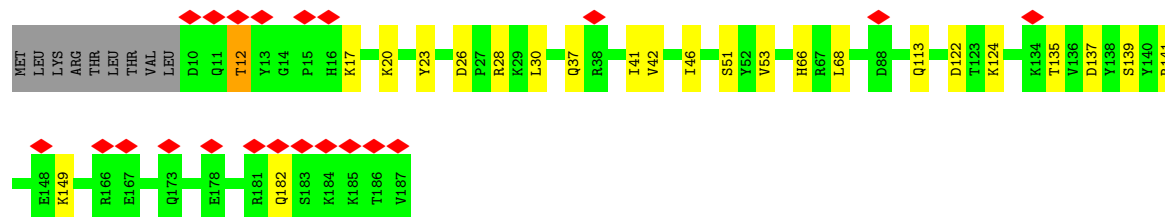
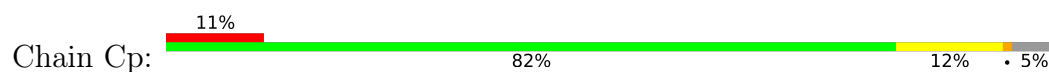
- Molecule 12: mS34



- Molecule 13: mS38

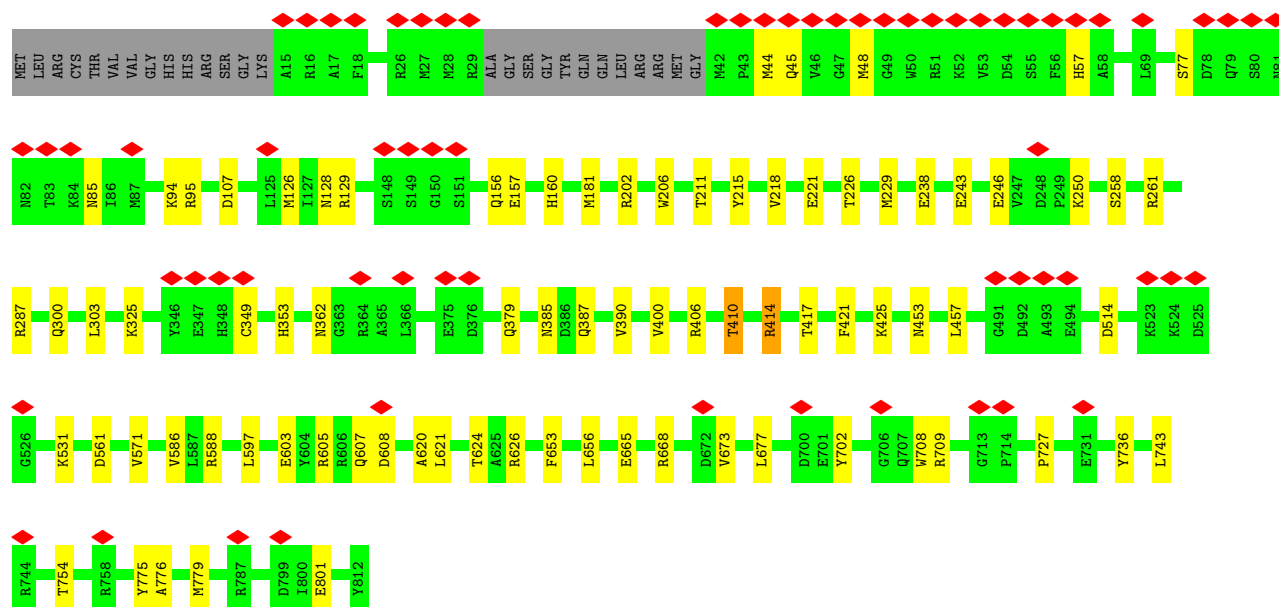


- Molecule 14: mS41

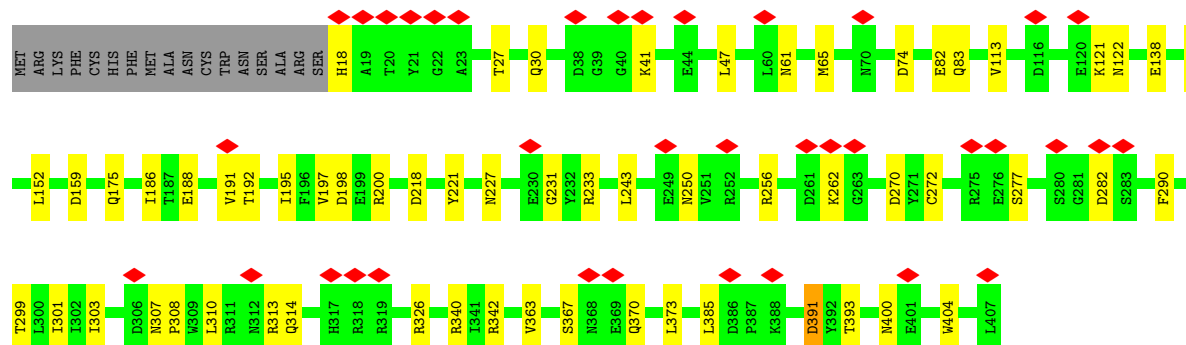
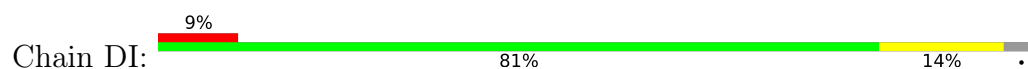


- Molecule 15: mS51 (KRIPP1)

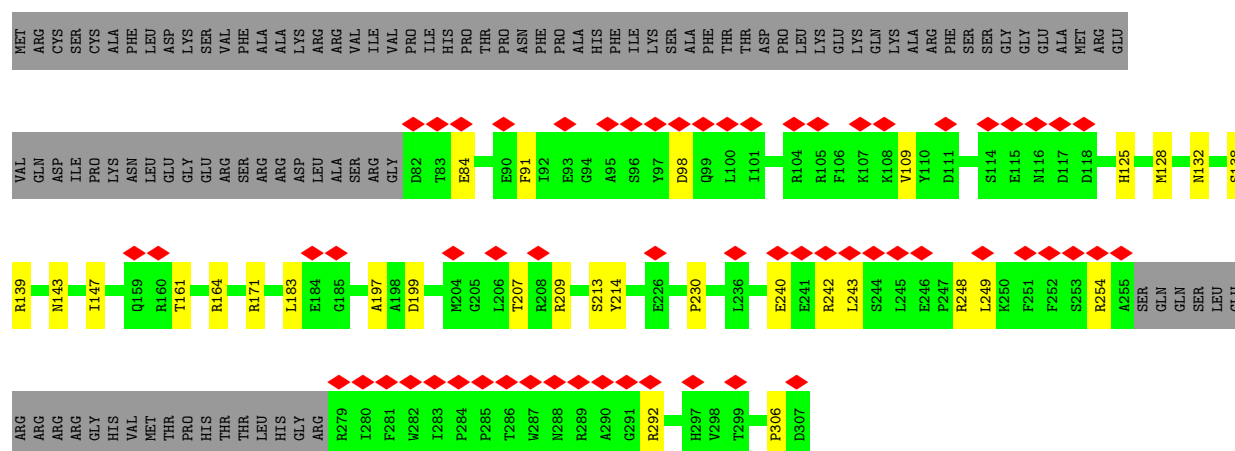




• Molecule 16: mS56



• Molecule 17: mS59

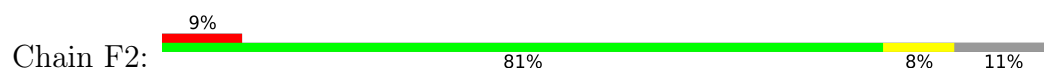




MET LEU ARG ARG SER ILE PHE MET LYS TYR ALA ASP LEU LEU THR ARG GLY GLU PHE PRO HIS GLY MET LYS GLU PRO ALA PHE VAL LYS LEU ASP GLN ASN ILE PRO THR PHE SER MET THR HIS TRP PRO ILE THR GLY ASP ASN TRP

SER ASP L63 M64 E65 A66 E67 K68 H69 D70 L72 W80 K81 K82 E85 G86 I87 F88 G89 V90 D91 E92 ASP SER

• Molecule 23: mt-SAF2 (KRIPP2)



MET LEU THR THR ARG LEU PRO K10 A11 P14 Q17 T28 K35 T46 P53 P54 V55 E64 R65 E77 Q78 D79 D80 I81 R87 N88 G99 R104 S105 E110 P111 L112 S113 A116 S117 K118 L119 Y120 V123 G124 ASP MET SER

GLY ASN THR ALA LEU PRO PRO ASN THR TYR ASP VAL LEU GLU GLN ASP VAL SER GLU MET ALA GLU ASP VAL VAL THR GLN PRO ARG LEU R165 A166 E167 K172 Y173 N174 M177 A178 D199 V200 E203 F204 T205 E206 D207 R218 I224 G225

R226 M235 G238 R245 E266 Q297 N301 M304 N307 V313 Q337 R352 L377 A378 H379 V387 V406 R417 D443 Y444 D445 E449 K450 D451 E460 R474 R475 V478 N485 D504 D532 Y536 D550 E551

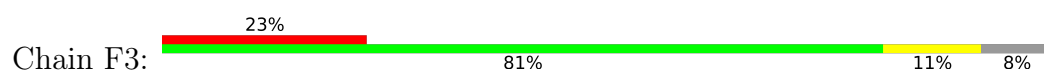
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L745 R751 E752 G754 E755 W763 D764 G765 G766 L768 D773 Q778 R786 E794 S809 T810 L811 Q830 T831 E834 D843 D847 G848 T848 L949 E953 E954 S955 E956 A960 S978 P979 Y980 D983 N982 T993 F994 L998 S999

THR GLU GLY LYS LEU SER ILE ALA LYS ALA MET GLN ASN LYS GLU GLN ASN VAL ASP VAL VAL ARG GLY LYS VAL T929 R930 K933 K939 V940 R941 H946 G947 T948 L949 E953 D964 K967 V974 R975 R982 K983 P985 A986 S987 E988 E989 L991

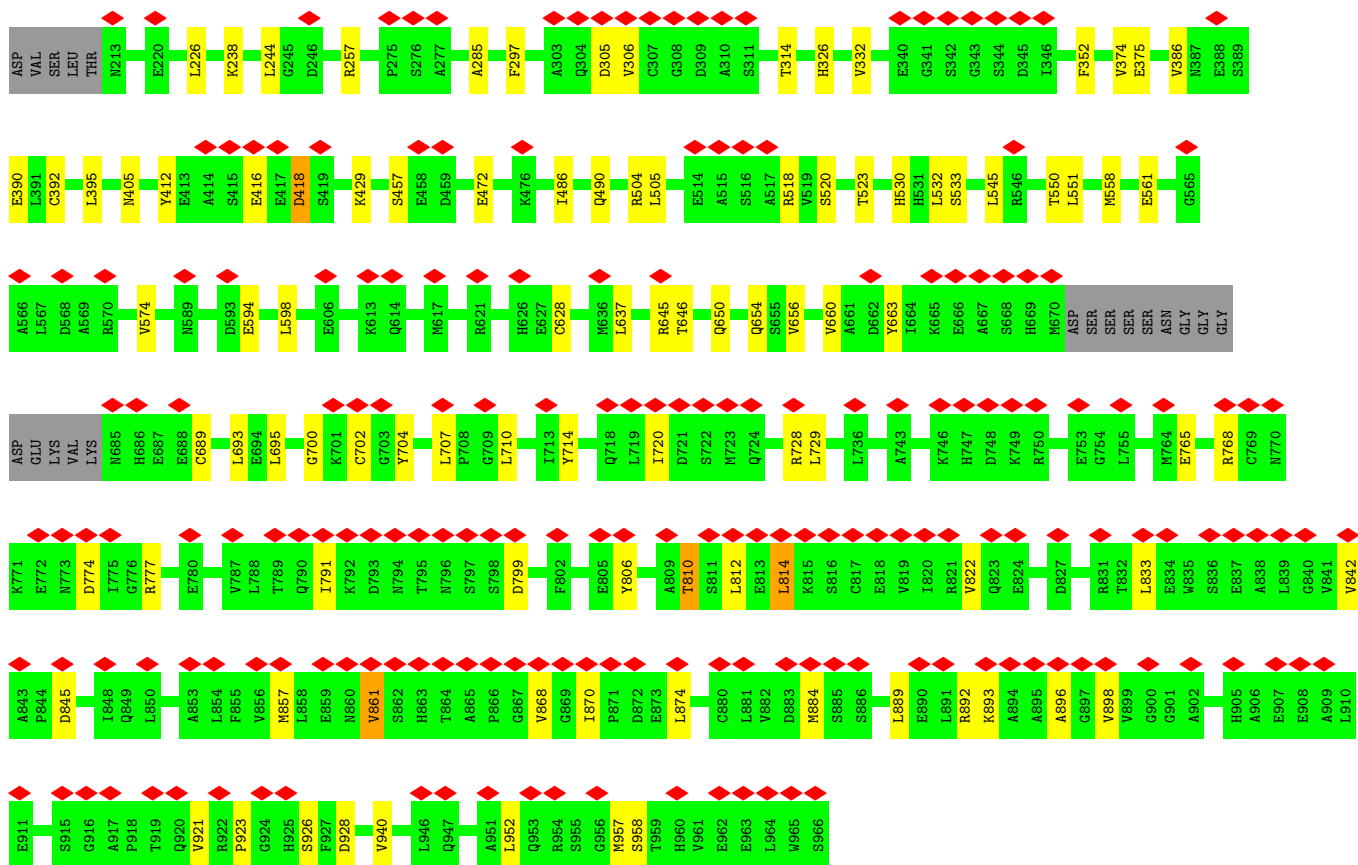
K992 R993 TRP ARG VAL ASP GLU GLN ARG SER ALA SER MET GLN THR VAL MET ALA SER ARG ALA LEU LYS LYS ARG LYS VAL ARG GLN VAL ARG SER HIS ARG ASN LYS

• Molecule 24: mt-SAF3

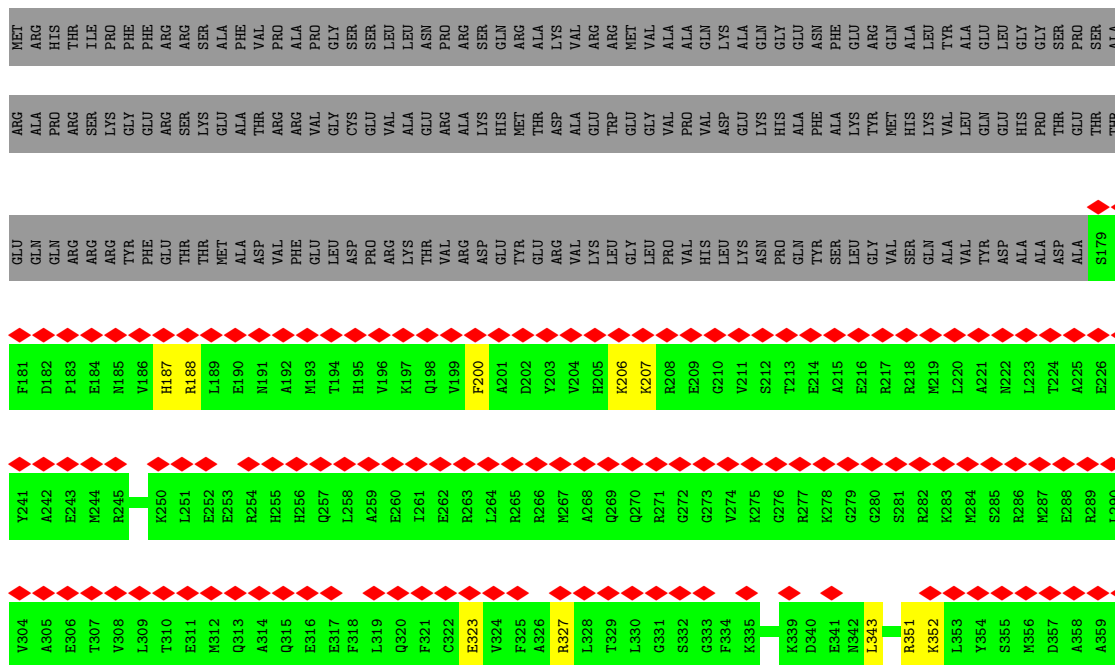


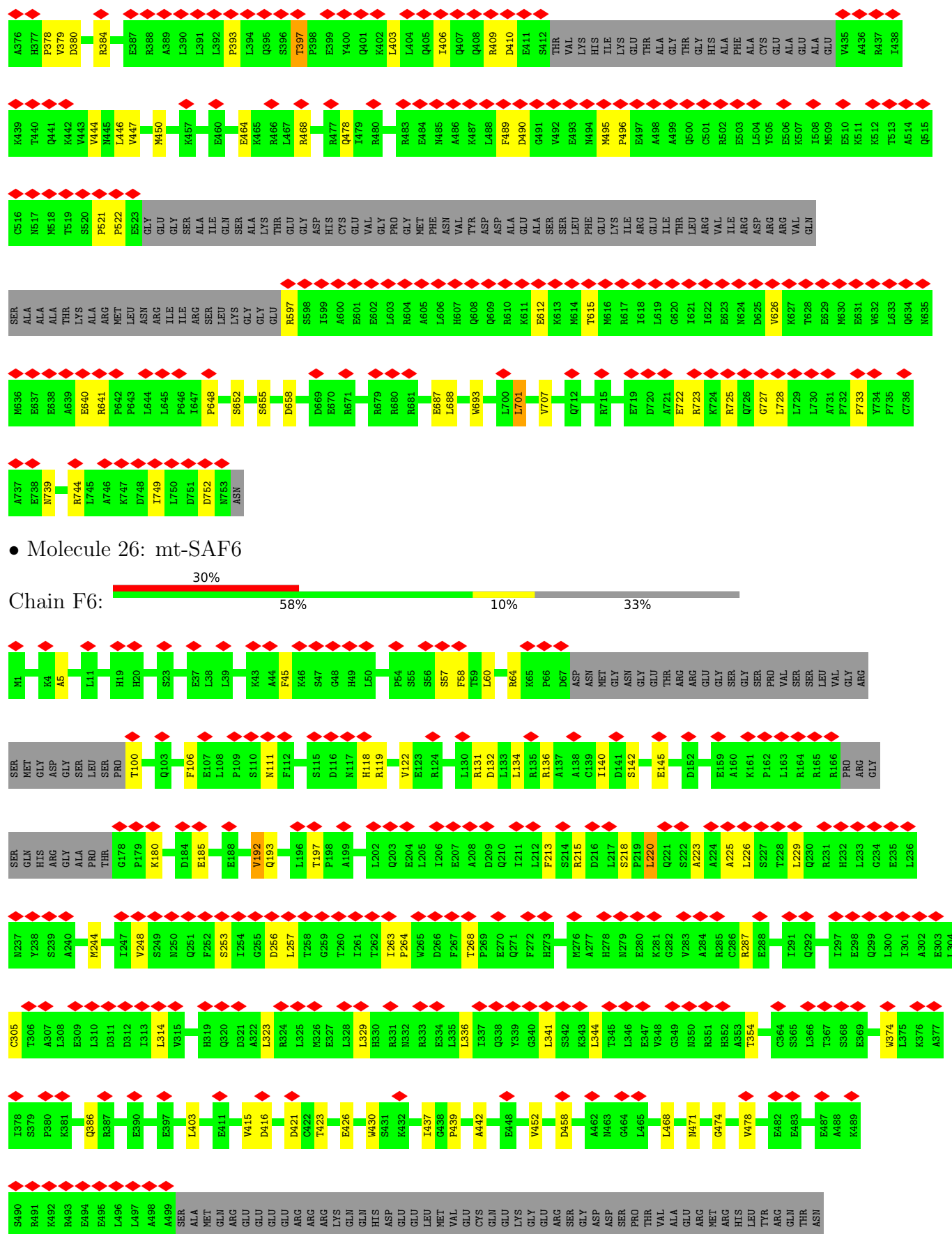
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L84 E85 S86 A87 A88 R92 E93 G102 D103 I104 E105 D106 D107 V112 D113 E114 R117 G118 G119 S120 S121 L122 T152 I153 N159 D163 Y164 E165 R169 R173 K174 R175 I180 R188 D194 V195 V196 GLU THR ALA ARG GLY ASP SER ALA GLN ALA



• Molecule 25: mt-SAF5

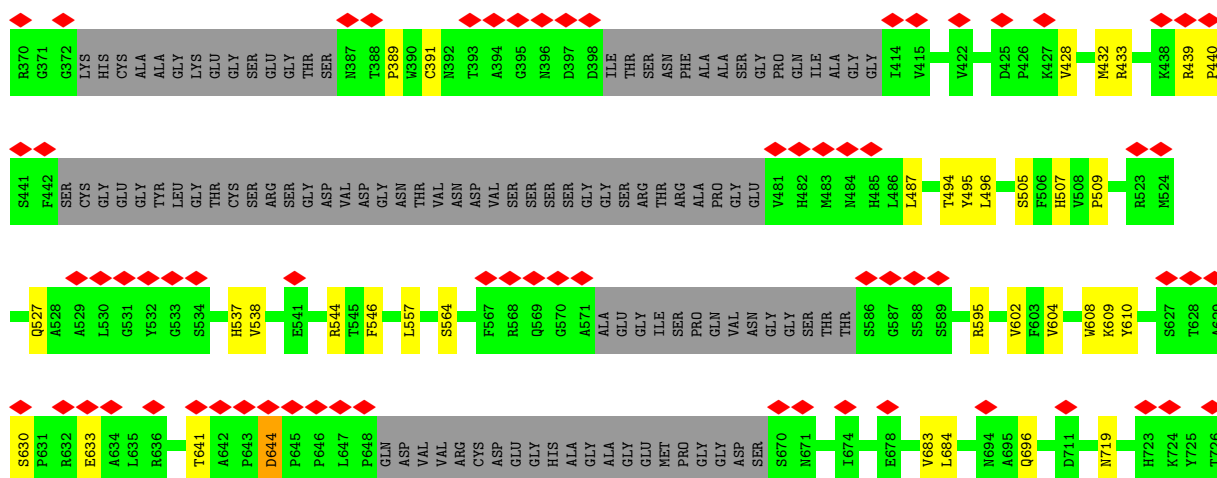




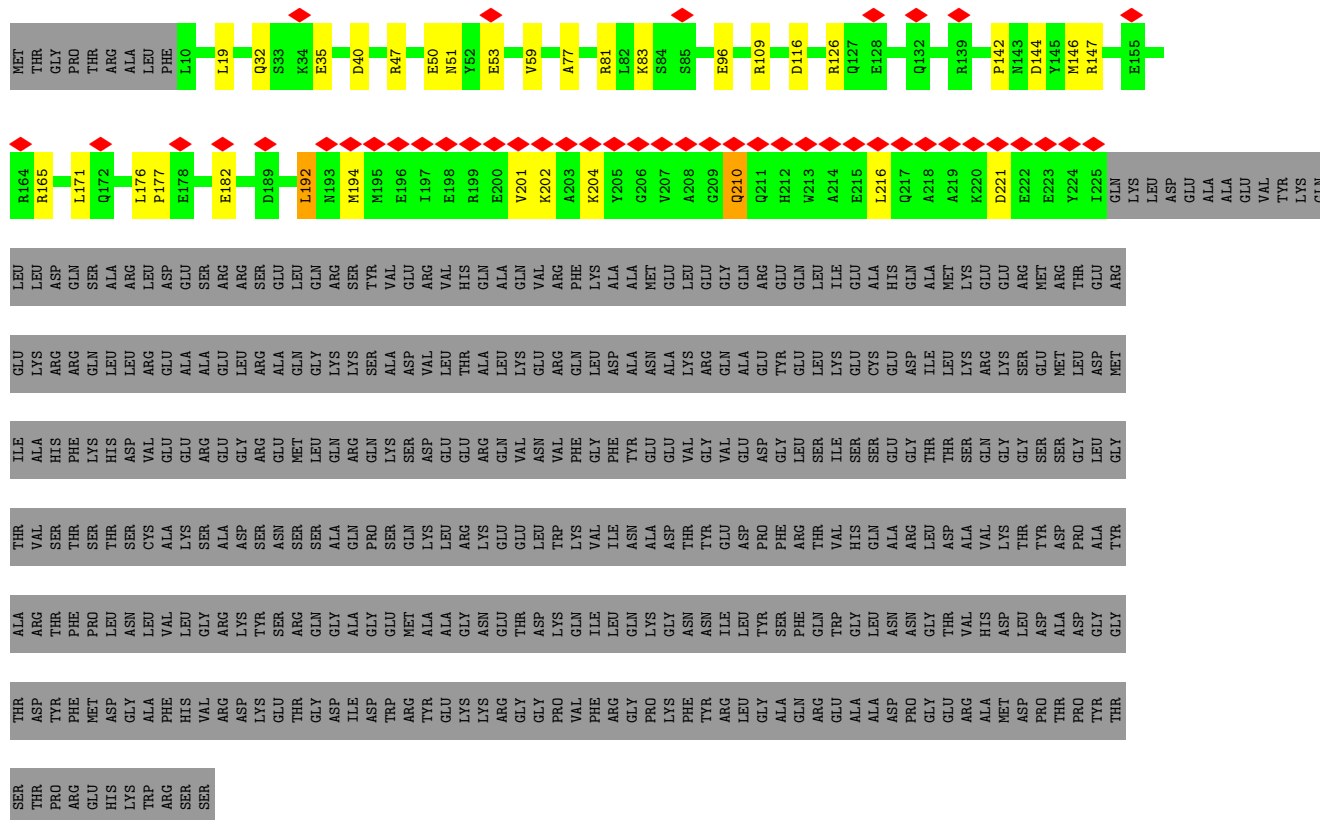
- Molecule 27: mt-SAF7 (KRIPP10)

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K655	V134	Q304	N450	SER
A656	D135	H308	M467	HIS
A657	K136	E309	E469	ALA
L658	L143	A310	C468	VAL
D659	L144	S311	A678	PRO
V660	P145	R312	T472	ARG
G661	T146	ALA	M475	LEU
S662	P147	THR	E476	R10
M663	G148	SER	L482	L11
R664	L149	GLU	E494	E20
R672	L155	GLY	S497	M26
V679	L158	ARG	A512	R27
	R178	Y321	R522	R28
	E181	L322	T532	K29
	A187	C323	N542	Q30
	Q190	E324	T555	K31
	V193	E327	L564	G32
	T202	E334	L565	D34
	N203	Q343	K566	V36
	T204	L351	I567	I36
	P205	E352	R568	R37
	P206	S377	C580	E38
	V207	D378	A583	K39
	E208	L379	E599	V40
	R237	R380	S600	D41
	E244	L381	L601	C42
	E247	S382	D604	T43
	E247	L383	S605	A44
	A265	F386	E606	W47
	V269	L389	K607	E52
	V279	D401	G608	Q53
	L284	R411	E609	N54
	R285	L424	A610	R63
	P286	L431	D614	L70
	R287	Q432	E615	L82
	M290	R433	P624	P87
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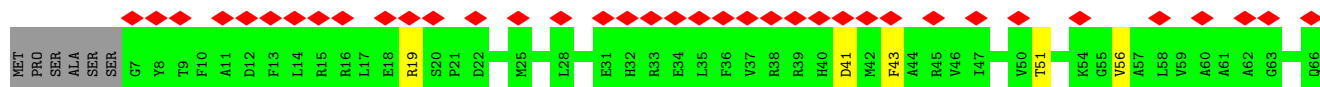
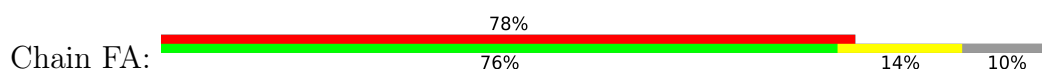
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	ASP	6	Green	S6
	GLY	7	Green	S7
	LEU	8	Green	S8
	LEU	9	Green	S9
	PRO	10	Green	S10
H	PRO	11	Green	H1
	SER	12	Green	H2
	HIS	13	Green	H3
	LEU	14	Green	H4
	LEU	15	Green	H5
	ALA	16	Green	H6
	ARG	17	Green	H7
	GLU	18	Green	H8
	LYS	19	Green	H9
	G	GLU	20	Green
LYS		21	Green	G2
ASP		22	Green	G3
ASN		23	Green	G4
ASP		24	Green	G5
GLY		25	Green	G6
ARG		26	Green	G7
PRO		27	Green	G8
SER		28	Green	G9
VAL		29	Green	G10
V	GLU	30	Green	V1
	GLY	31	Green	V2
	V303	32	Green	V303
	A304	33	Green	A304
	A309	34	Green	A309
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	Q328	36	Green	Q328
	R329	37	Green	R329
	G330	38	Green	G330
	VAL	39	Green	V39
A	ASP	40	Green	A40
	GLY	41	Green	A41
	THR	42	Green	A42
	ALA	43	Green	A43
	SER	44	Green	A44
	ARG	45	Green	A45
	GLY	46	Green	A46
	GLY	47	Green	A47
	ASN	48	Green	A48
	ASP	49	Green	A49
E	ASP	50	Green	E50
	D245	51	Green	D245
	H248	52	Green	H248
	H249	53	Green	H249
	L250	54	Green	L250
	H257	55	Green	H257
	D262	56	Green	D262
	S268	57	Green	S268
	R269	58	Green	R269
	GLU	59	Green	GLU
T	ALA	60	Green	T60
	ALA	61	Green	T61
	S352	62	Green	S352
	T353	63	Green	T353
	GLY	64	Green	T64
	THR	65	Green	T65
	CYS	66	Green	T66
	ASN	67	Green	T67
	GLY	68	Green	T68
	GLY	69	Green	T69
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	ALA	73	Green	M73
	SER	74	Green	M74
	ASN	75	Green	M75
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	GLY	79	Green	M79
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	VAL	81	Green	I81
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	GLY	86	Green	I86
	GLY	87	Green	I87
	GLY	88	Green	I88
	GLY	89	Green	I89
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	ALA	93	Green	R93
	SER	94	Green	R94
	ASN	95	Green	R95
	GLY	96	Green	R96
	GLY	97	Green	R97
	GLY	98	Green	R98
	GLY	99	Green	R99
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	THR	102	Green	Y102
	ALA	103	Green	Y103
	SER	104	Green	Y104
	ASN	105	Green	Y105
	GLY	106	Green	Y106
	GLY	107	Green	Y107
	GLY	108	Green	Y108
	GLY	109	Green	Y109
MET	ASP	110	Green	MET110
	VAL	111	Green	MET111
	THR	112	Green	MET112
	ALA	113	Green	MET113
	SER	114	Green	MET114
	ASN	115	Green	MET115
	GLY	116	Green	MET116
	GLY	117	Green	MET117
	GLY	118	Green	MET118
	GLY	119	Green	MET119

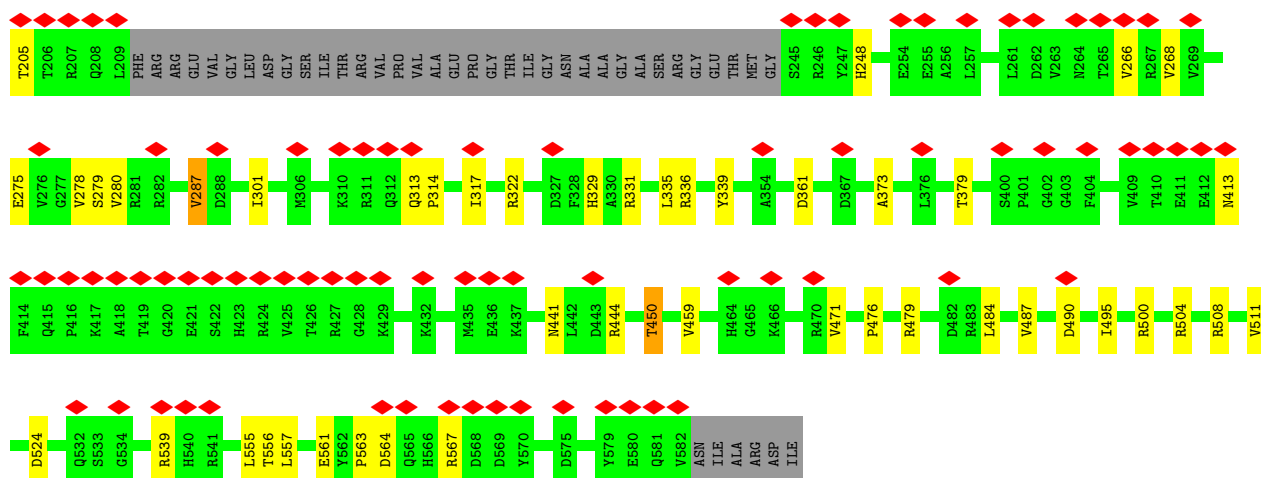


• Molecule 29: mt-SAF9

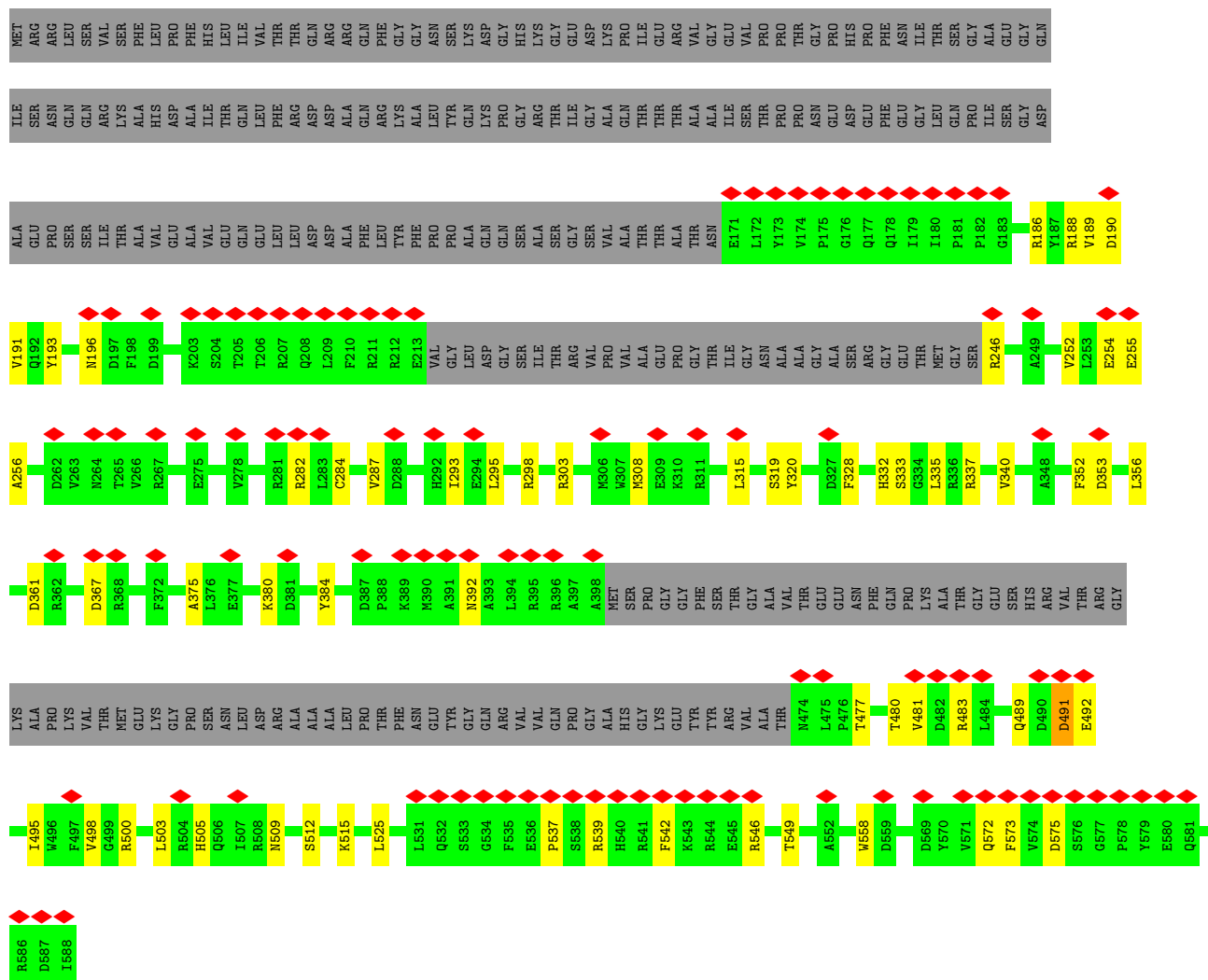
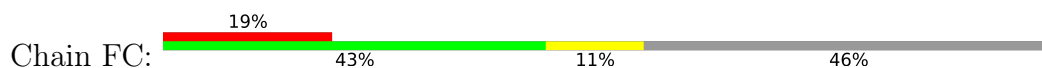


• Molecule 30: mt-SAF10

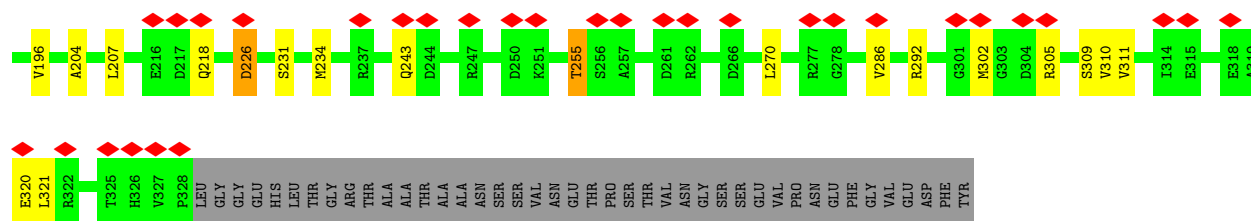




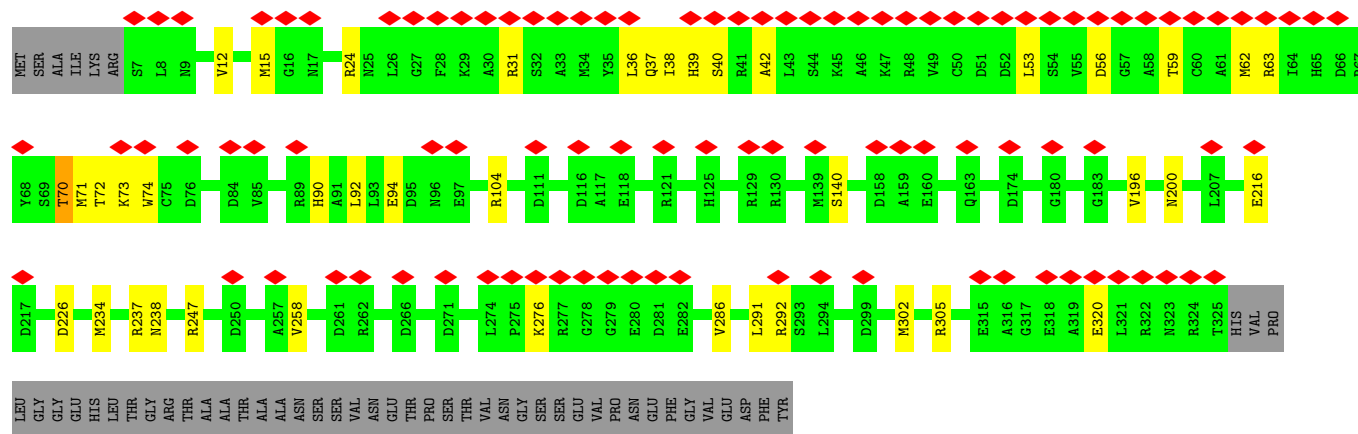
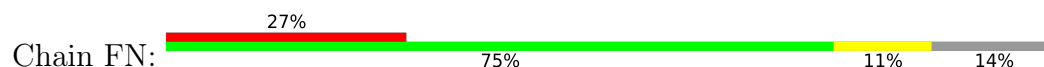
• Molecule 31: mt-SAF11



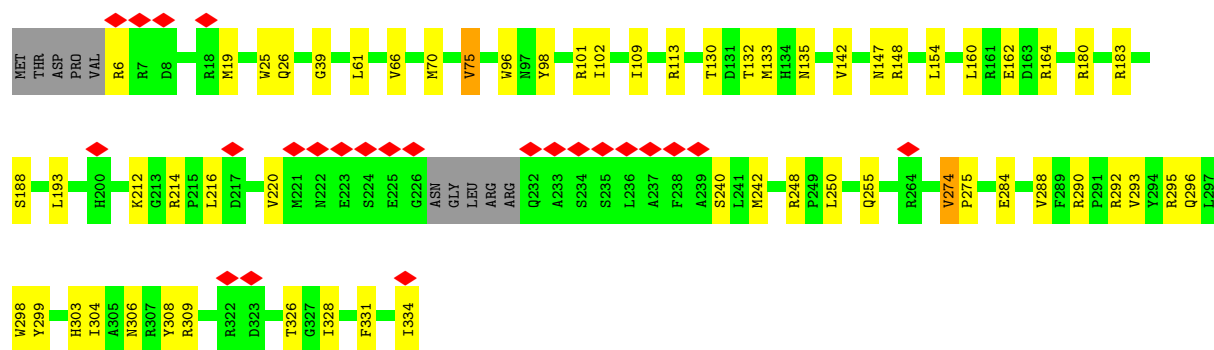
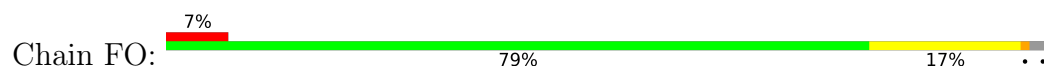
• Molecule 32: mt-SAF13



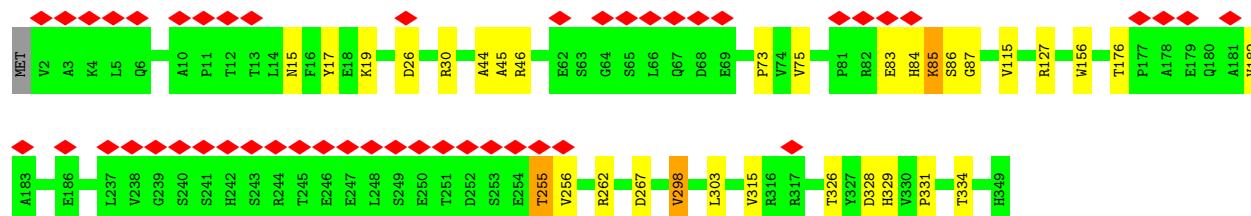
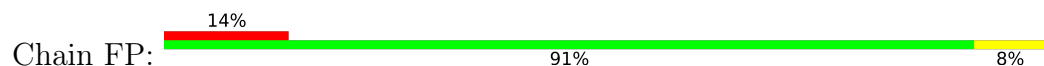
• Molecule 34: mt-SAF21



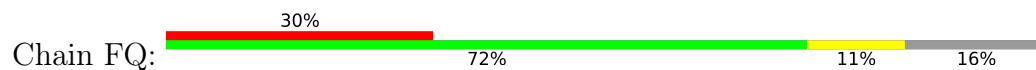
• Molecule 35: mt-SAF22 (KRIPP17)



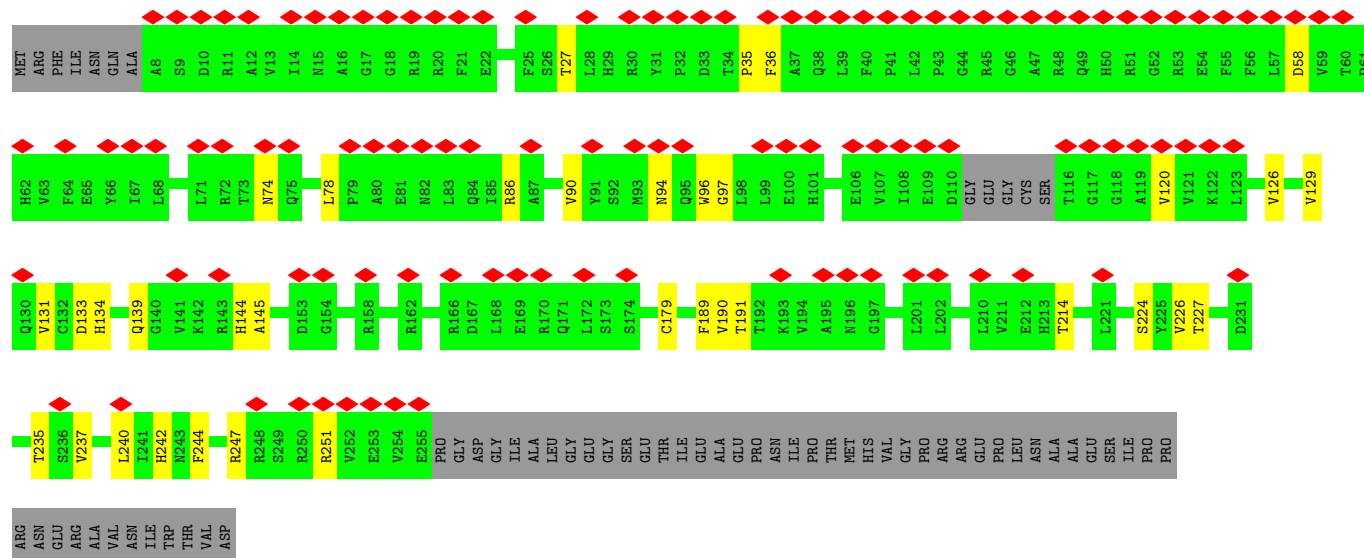
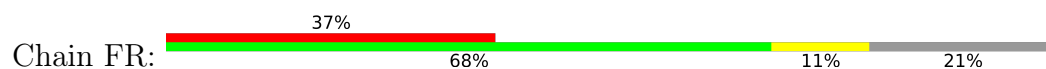
• Molecule 36: mt-SAF23



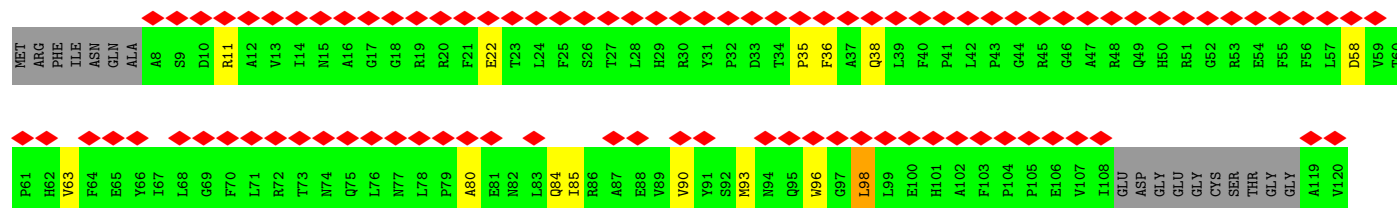
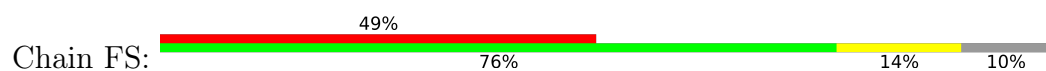
- Molecule 37: mt-SAF24

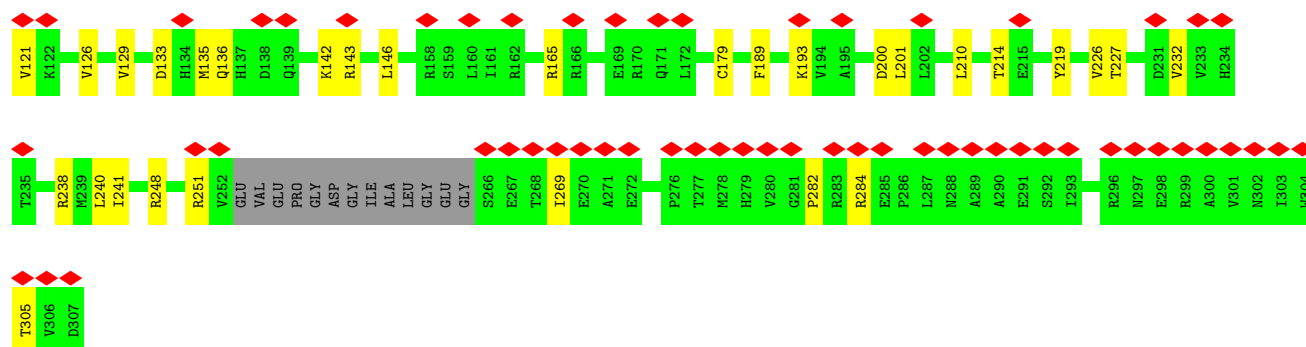


- Molecule 37: mt-SAF24

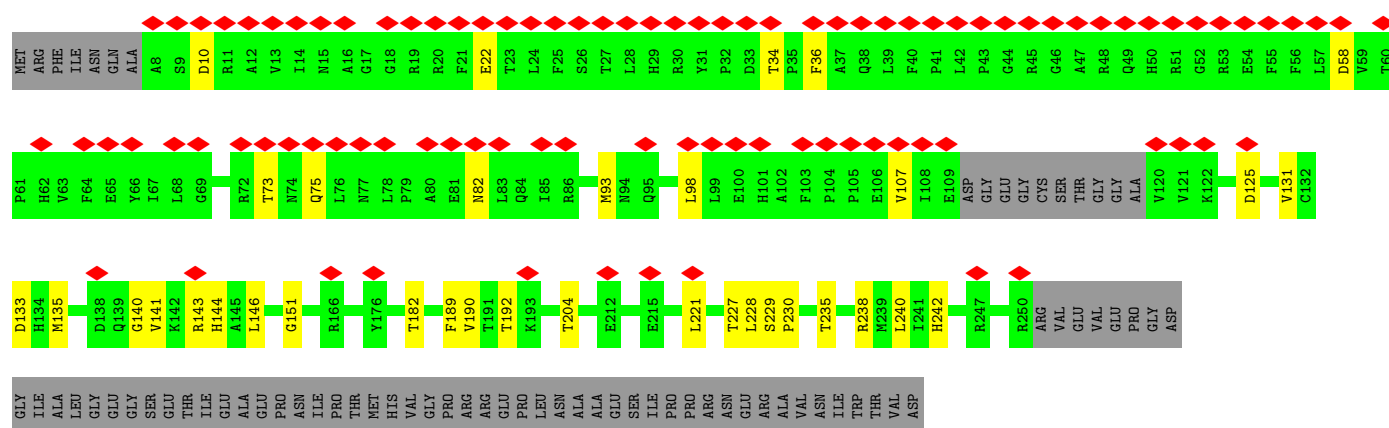


- Molecule 37: mt-SAF24

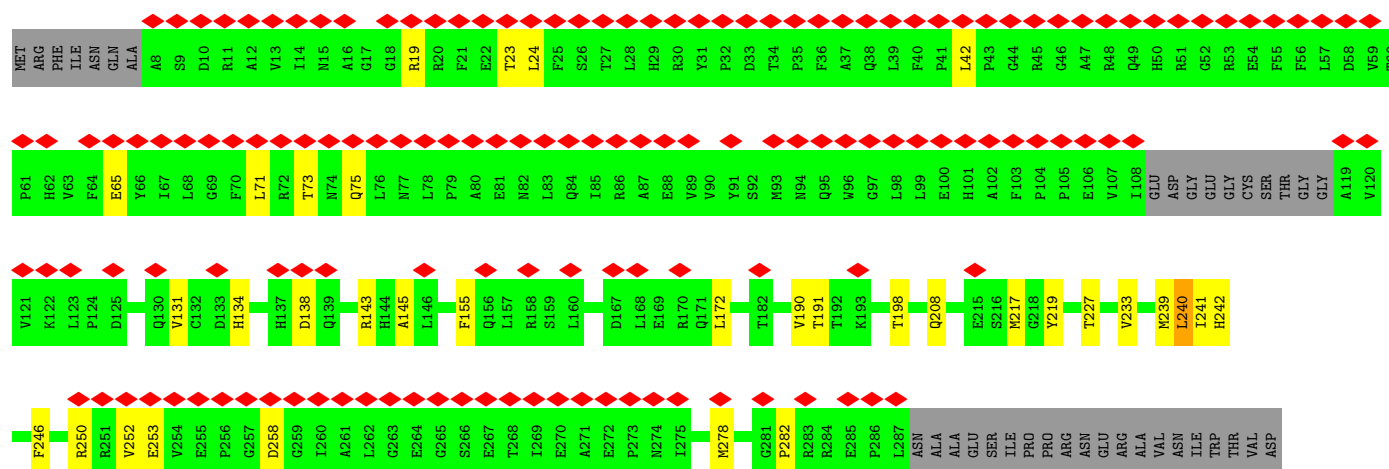
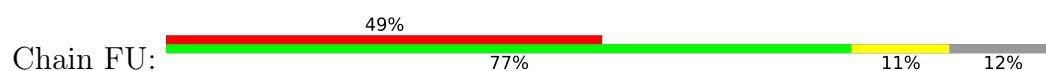




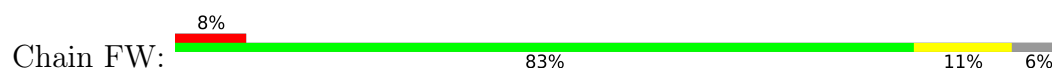
• Molecule 37: mt-SAF24

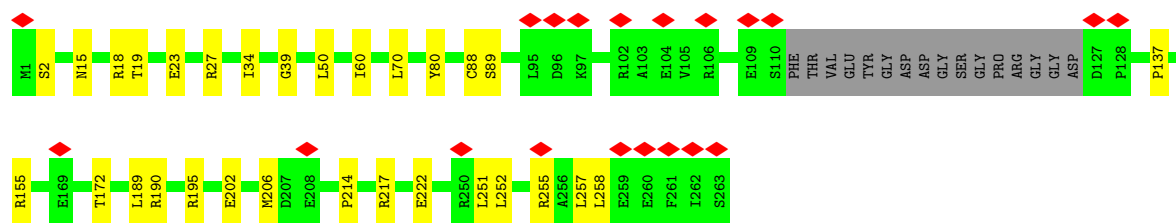


• Molecule 37: mt-SAF24



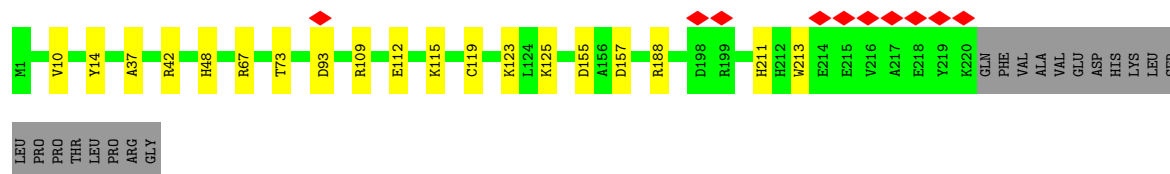
• Molecule 38: mt-SAF26





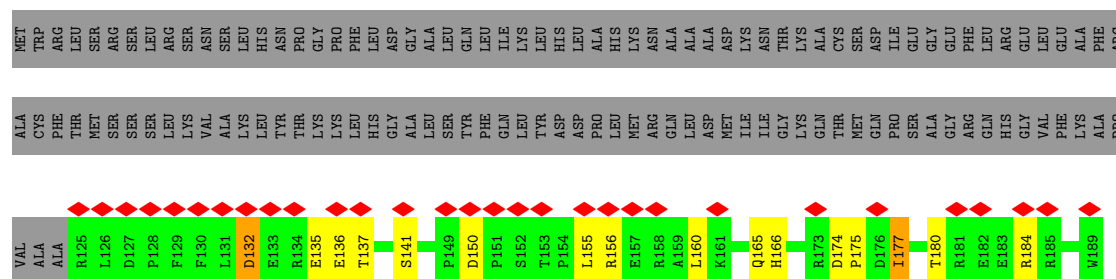
• Molecule 39: mt-SAF27

Chain FX: 84% 8% 8%



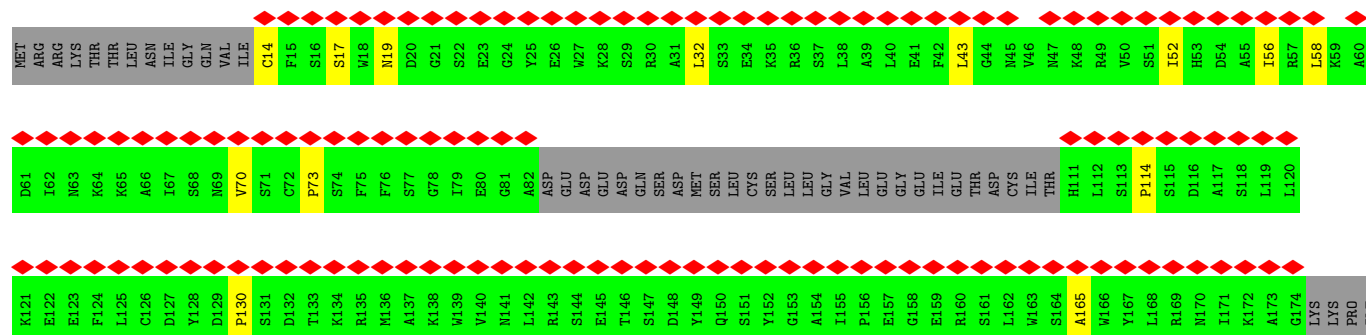
• Molecule 40: mt-SAF28

Chain FY: 16% 26% 7% 65%



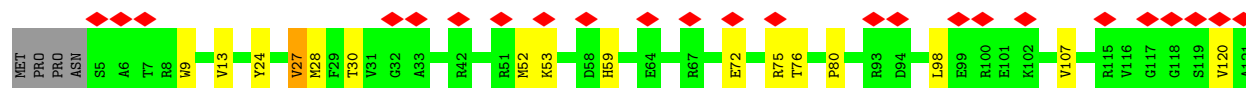
• Molecule 41: mt-SAF29

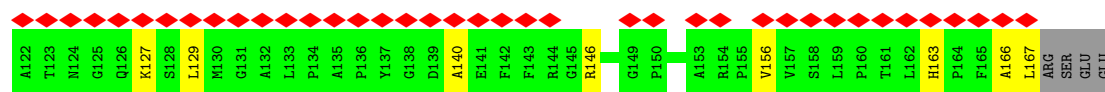
Chain FZ: 74% 67% 7% 25%



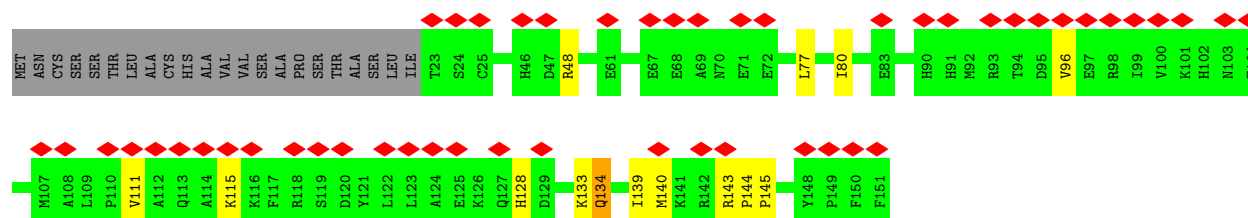
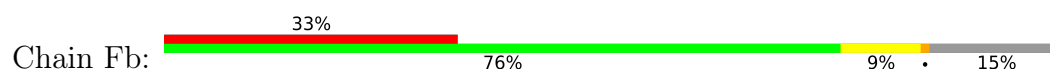
• Molecule 42: mt-SAF30

Chain Fa: 37% 81% 13% 5%

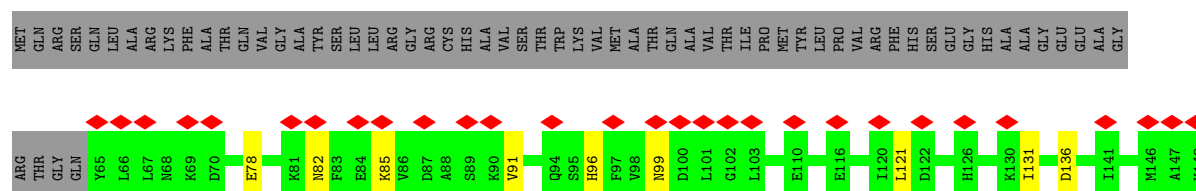




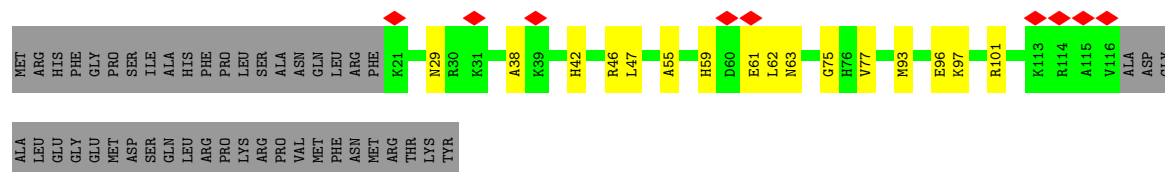
• Molecule 43: mt-SAF31



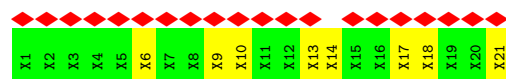
• Molecule 44: mt-SAF32



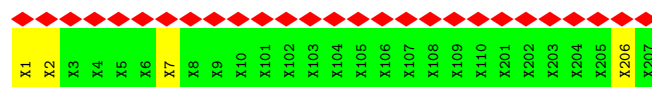
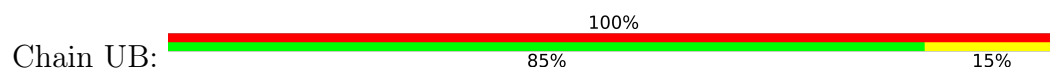
• Molecule 45: mt-SAF33



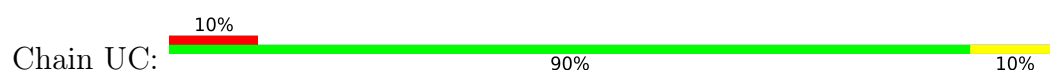
• Molecule 46: UNK-A



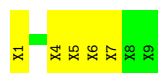
• Molecule 47: UNK-B



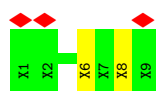
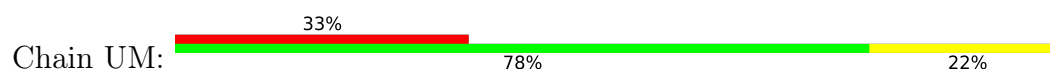
• Molecule 48: UNK-C



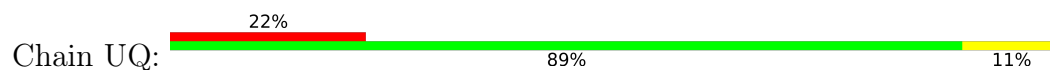
- Molecule 49: UNK-D, UNK-M, UNK-Q



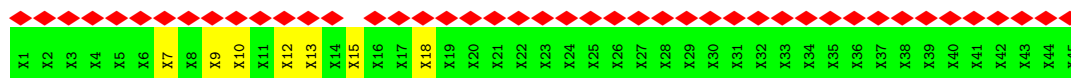
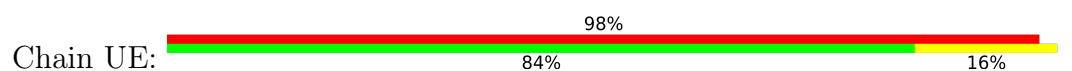
- Molecule 49: UNK-D, UNK-M, UNK-Q



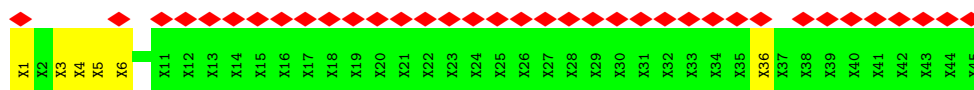
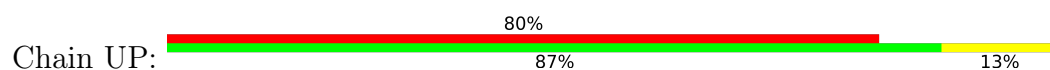
- Molecule 49: UNK-D, UNK-M, UNK-Q



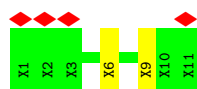
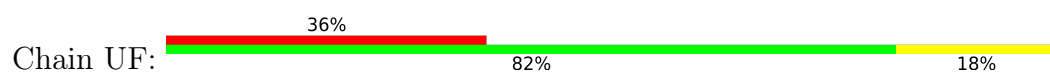
- Molecule 50: UNK-E, UNK-P



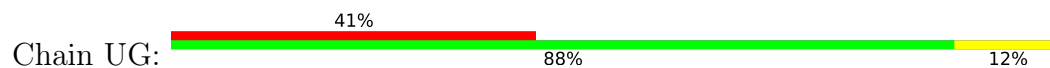
- Molecule 50: UNK-E, UNK-P



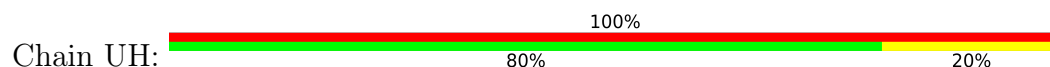
- Molecule 51: UNK-F



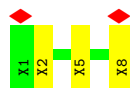
• Molecule 52: UNK-G



• Molecule 53: UNK-H



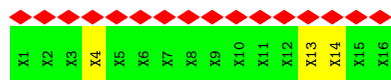
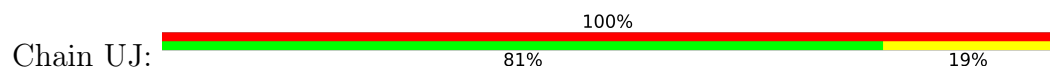
• Molecule 54: UNK-I, UNK-M



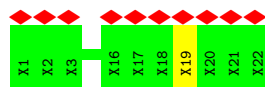
• Molecule 54: UNK-I, UNK-M



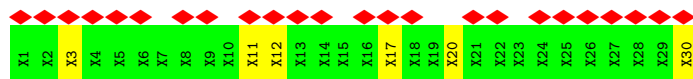
• Molecule 55: UNK-J



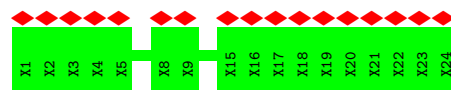
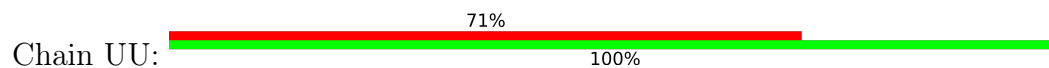
• Molecule 56: UNK-L



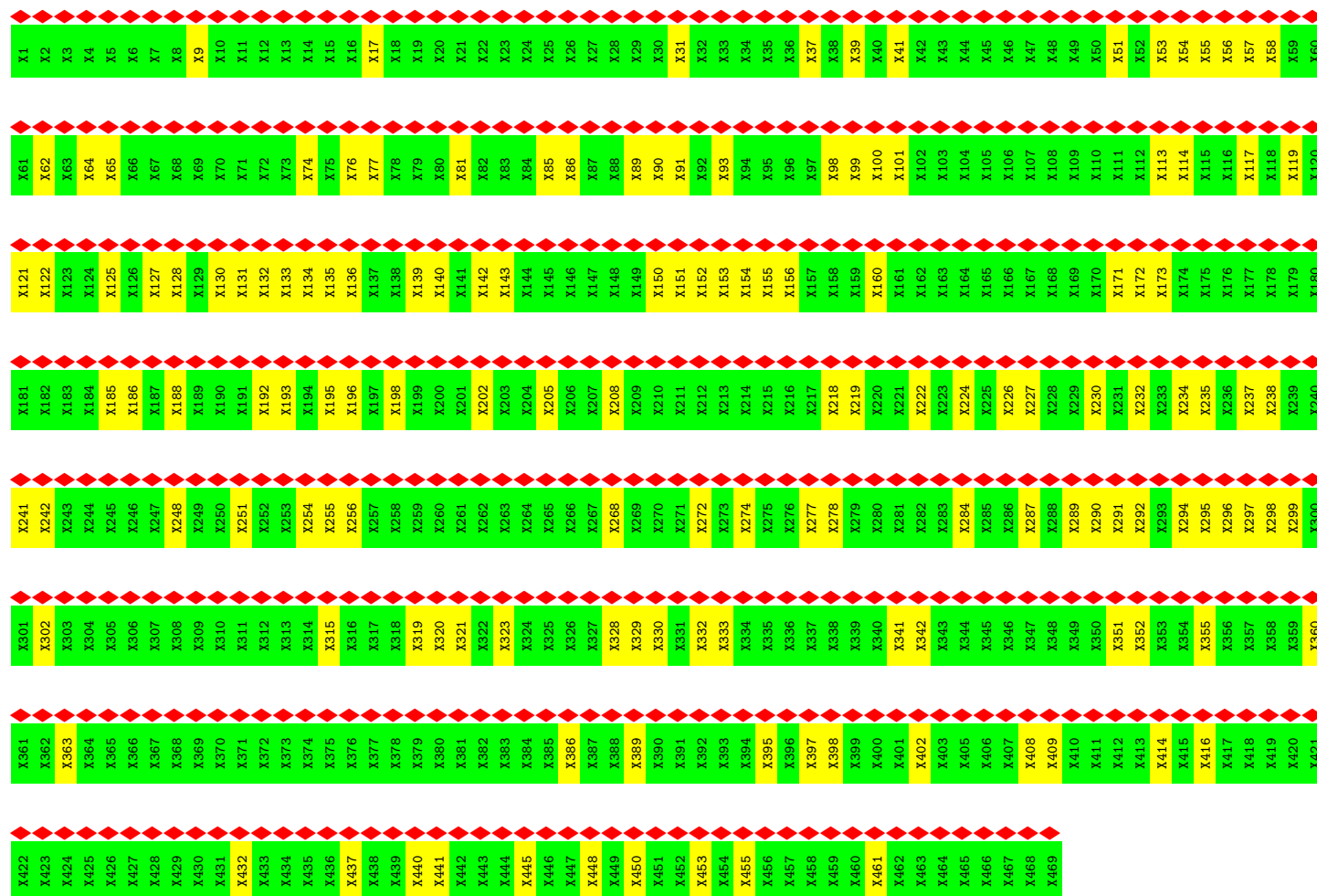
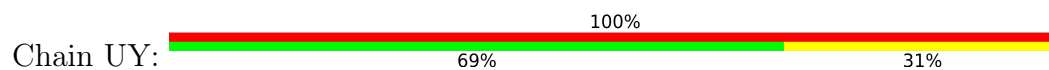
• Molecule 57: UNK-O



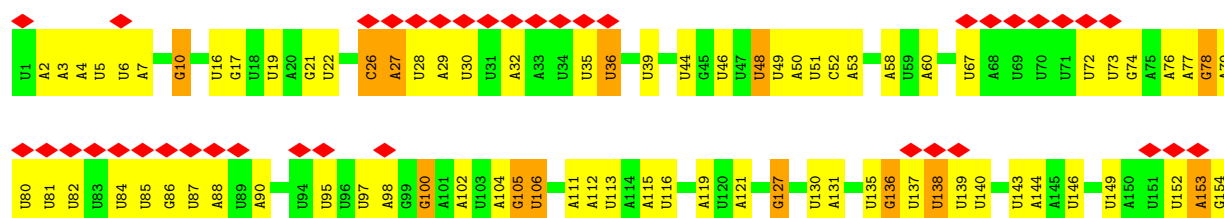
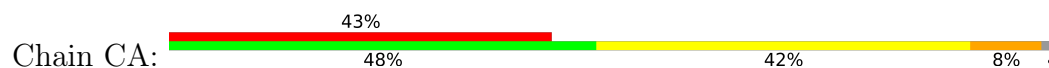
● Molecule 58: UNK-U

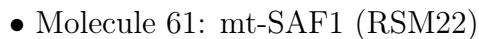


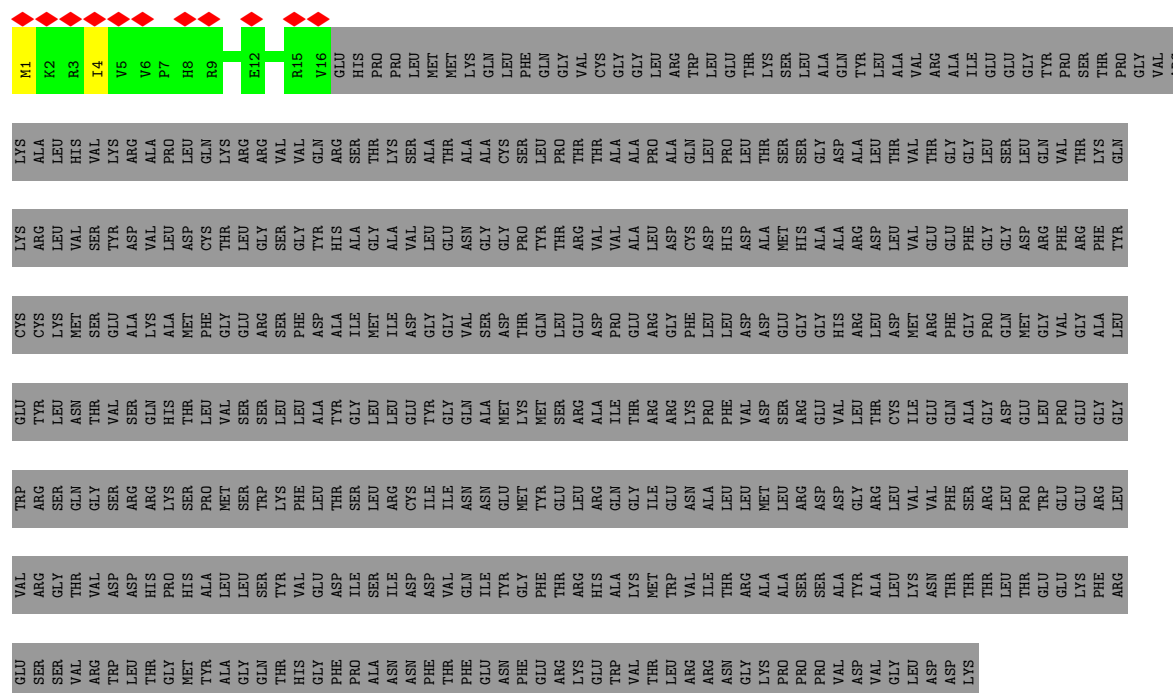
● Molecule 59: UNK-I



● Molecule 60: 9S rRNA



[illegible]



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	161661	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; On the fly in RELION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	100719	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.455	Depositor
Minimum map value	-0.193	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.0902	Depositor
Map size (Å)	333.6, 333.6, 333.6	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PM8, PO4, UBD, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	CE	0.15	0/3226	0.42	1/4364 (0.0%)
2	CF	0.13	0/1344	0.33	0/1813
3	CH	0.16	0/1864	0.41	0/2511
4	CK	0.15	0/1417	0.39	0/1911
5	CO	0.15	0/3057	0.38	0/4121
6	CP	0.16	0/1533	0.42	0/2074
7	CQ	0.15	0/1856	0.39	0/2509
8	CR	0.15	0/1315	0.42	0/1785
9	Ca	0.16	0/4474	0.41	1/6052 (0.0%)
10	Cb	0.16	0/1304	0.39	0/1751
11	Cd	0.23	0/1662	0.37	0/2234
12	Cj	0.14	0/1842	0.37	0/2511
13	Cn	0.18	0/245	0.52	0/333
14	Cp	0.13	0/1551	0.35	0/2103
15	DD	0.15	0/6678	0.38	0/9051
16	DI	0.14	0/3248	0.34	0/4401
17	DL	0.15	0/1699	0.39	0/2293
18	DO	0.12	0/1680	0.33	0/2265
19	DP	0.14	0/1854	0.36	0/2511
20	DR	0.16	0/2107	0.40	0/2871
21	DU	0.15	0/1780	0.47	2/2416 (0.1%)
22	DZ	0.12	0/263	0.31	0/355
23	F2	0.16	0/7432	0.39	2/10042 (0.0%)
24	F3	0.16	0/6999	0.40	4/9472 (0.0%)
25	F5	0.18	0/3533	0.42	3/4798 (0.1%)
26	F6	0.16	0/3728	0.42	0/5060
27	F7	0.17	0/5342	0.44	1/7236 (0.0%)
28	F8	0.14	0/4025	0.36	0/5450
29	F9	0.15	0/1785	0.34	0/2399
30	FA	0.18	0/4507	0.42	0/6139
31	FB	0.14	0/3132	0.37	0/4248
31	FC	0.15	0/2635	0.40	0/3572

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	FE	0.14	0/3629	0.36	0/4935
33	FJ	0.15	0/2986	0.41	0/4030
34	FM	0.16	0/2489	0.37	0/3365
34	FN	0.15	0/2430	0.38	0/3285
35	FO	0.16	0/2733	0.41	0/3692
36	FP	0.16	0/2710	0.41	2/3709 (0.1%)
37	FQ	0.14	0/2048	0.34	0/2786
37	FR	0.13	0/1966	0.34	0/2673
37	FS	0.13	0/2249	0.33	0/3063
37	FT	0.13	0/1897	0.33	0/2580
37	FU	0.14	0/2154	0.35	0/2933
38	FW	0.13	0/2077	0.35	0/2805
39	FX	0.15	0/1783	0.38	0/2410
40	FY	0.17	0/562	0.48	0/769
41	FZ	0.14	0/989	0.49	3/1336 (0.2%)
42	Fa	0.14	0/1363	0.39	0/1853
43	Fb	0.14	0/1123	0.39	0/1513
44	Fc	0.11	0/679	0.27	0/923
45	Fd	0.15	0/779	0.37	0/1054
60	CA	0.15	0/9830	0.37	1/15261 (0.0%)
61	F1	0.16	0/469	0.40	0/624
62	FF	0.11	0/144	0.28	0/192
All	All	0.15	0/136206	0.39	20/186442 (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
15	DD	0	1
24	F3	0	1
27	F7	0	2
28	F8	0	1
36	FP	0	1
38	FW	0	1
All	All	0	7

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Ca	525	PRO	N-CA-CB	10.89	110.53	103.23
1	CE	385	PRO	N-CA-CB	8.20	111.86	103.25
21	DU	206	PRO	N-CA-CB	7.98	110.39	103.36
21	DU	200	PRO	N-CA-CB	7.52	110.33	103.19
25	F5	521	PRO	N-CA-CB	7.32	110.18	103.08
41	FZ	130	PRO	N-CA-CB	7.25	110.20	103.46
25	F5	496	PRO	N-CA-CB	6.91	110.63	103.38
23	F2	946	HIS	CA-C-N	6.85	134.02	121.70
23	F2	946	HIS	C-N-CA	6.85	134.02	121.70
41	FZ	73	PRO	N-CA-CB	6.83	110.42	103.25
25	F5	522	PRO	N-CA-CB	6.29	110.18	103.52
41	FZ	114	PRO	N-CA-CB	6.24	110.13	103.52
24	F3	702	CYS	CA-C-N	6.10	132.69	121.70
24	F3	702	CYS	C-N-CA	6.10	132.69	121.70
60	CA	349	U	P-O3'-C3'	5.34	128.21	120.20
24	F3	645	ARG	CA-C-N	5.24	131.55	121.54
24	F3	645	ARG	C-N-CA	5.24	131.55	121.54
36	FP	83	GLU	CA-C-N	5.20	131.46	121.54
36	FP	83	GLU	C-N-CA	5.20	131.46	121.54
27	F7	382	SER	N-CA-C	5.05	117.33	111.02

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	DD	414	ARG	Peptide
24	F3	490	GLN	Peptide
27	F7	381	LEU	Peptide
27	F7	566	LYS	Peptide
28	F8	644	ASP	Peptide
36	FP	84	HIS	Peptide
38	FW	214	PRO	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	CE	3147	0	3091	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	CF	1317	0	1309	21	0
3	CH	1824	0	1800	18	0
4	CK	1384	0	1361	13	0
5	CO	2979	0	2974	34	0
6	CP	1489	0	1510	14	0
7	CQ	1805	0	1811	33	0
8	CR	1274	0	1223	18	0
9	Ca	4340	0	4127	55	0
10	Cb	1274	0	1287	17	0
11	Cd	1616	0	1568	23	0
12	Cj	1792	0	1744	21	0
13	Cn	234	0	222	0	0
14	Cp	1506	0	1467	17	0
15	DD	6488	0	6251	60	0
16	DI	3182	0	3153	43	0
17	DL	1656	0	1632	16	0
18	DO	1648	0	1615	13	0
19	DP	1800	0	1765	14	0
20	DR	2042	0	2043	26	0
21	DU	1738	0	1640	15	0
22	DZ	254	0	230	8	0
23	F2	7274	0	7113	53	0
24	F3	6879	0	6854	55	0
25	F5	3474	0	3070	35	0
26	F6	3646	0	3608	38	0
27	F7	5225	0	5177	59	0
28	F8	3934	0	3908	35	0
29	F9	1755	0	1709	21	0
30	FA	4421	0	4534	45	0
31	FB	3055	0	3011	32	0
31	FC	2572	0	2544	33	0
32	FE	3523	0	3460	44	0
33	FJ	2917	0	2966	25	0
34	FM	2449	0	2440	26	0
34	FN	2392	0	2375	20	0
35	FO	2671	0	2636	44	0
36	FP	2643	0	2554	16	0
37	FQ	2003	0	1928	19	0
37	FR	1923	0	1862	19	0
37	FS	2198	0	2142	26	0
37	FT	1854	0	1802	20	0
37	FU	2105	0	2031	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	FW	2034	0	2035	19	0
39	FX	1741	0	1693	14	0
40	FY	544	0	533	13	0
41	FZ	973	0	869	8	0
42	Fa	1323	0	1336	12	0
43	Fb	1091	0	1085	12	0
44	Fc	669	0	663	4	0
45	Fd	758	0	764	11	0
46	UA	126	0	128	9	0
47	UB	162	0	169	4	0
48	UC	60	0	63	1	0
49	UD	54	0	57	6	0
49	UM	54	0	57	3	0
49	UQ	54	0	56	1	0
50	UE	270	0	272	5	0
50	UP	270	0	272	7	0
51	UF	66	0	69	2	0
52	UG	102	0	104	2	0
53	UH	30	0	33	1	0
54	UI	48	0	50	3	0
54	UN	48	0	50	4	0
55	UJ	96	0	99	2	0
56	UL	132	0	134	1	0
57	UO	180	0	183	8	0
58	UU	144	0	147	0	0
59	UY	2808	0	2852	102	0
60	CA	8851	0	4424	80	0
61	F1	465	0	492	3	0
62	FF	141	0	151	3	0
63	CAA	1	0	0	0	0
63	CAB	1	0	0	0	0
63	FPA	1	0	0	0	0
63	FWB	1	0	0	0	0
64	FWA	5	0	0	1	0
65	FcA	32	0	39	1	0
66	FdA	1	0	0	0	0
All	All	137038	0	130426	1190	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (1190) 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)
59:UY:355:UNK:HG1	60:CA:579:G:H5'	1.61	0.82
27:F7:206:PRO:HB3	59:UY:193:UNK:HB1	1.62	0.81
59:UY:9:UNK:HG1	59:UY:461:UNK:HB2	1.63	0.81
41:FZ:14:CYS:N	41:FZ:17:SER:HG	1.82	0.77
59:UY:351:UNK:HB1	60:CA:542:G:H5'	1.68	0.76
59:UY:272:UNK:HB1	59:UY:294:UNK:HB1	1.67	0.75
60:CA:100:G:H1	60:CA:127:G:HO2'	1.34	0.70
9:Ca:405:ARG:HE	15:DD:776:ALA:HB1	1.57	0.70
59:UY:153:UNK:HB2	59:UY:299:UNK:HG1	1.74	0.69
27:F7:128:ASP:HB3	59:UY:298:UNK:HB1	1.74	0.69
59:UY:160:UNK:HG3	59:UY:450:UNK:HG2	1.75	0.68
55:UJ:13:UNK:HG2	55:UJ:14:UNK:HG3	1.74	0.68
59:UY:51:UNK:HG3	59:UY:65:UNK:HG1	1.76	0.68
59:UY:99:UNK:HB1	59:UY:130:UNK:HB1	1.75	0.68
59:UY:153:UNK:HG2	59:UY:296:UNK:HB1	1.76	0.68
45:Fd:38:ALA:HA	45:Fd:42:HIS:HB2	1.77	0.66
31:FB:279:SER:HB2	31:FB:556:THR:HG22	1.78	0.66
26:F6:57:SER:HA	26:F6:106:PHE:O	1.96	0.66
59:UY:192:UNK:HG2	59:UY:193:UNK:HG2	1.78	0.66
32:FE:432:HIS:HB3	32:FE:439:PRO:HB3	1.77	0.66
39:FX:119:CYS:HB2	54:UN:1:UNK:H2	1.60	0.65
59:UY:332:UNK:HG2	59:UY:333:UNK:HG3	1.78	0.65
59:UY:90:UNK:HG3	59:UY:91:UNK:HG3	1.79	0.65
46:UA:17:UNK:HG2	57:UO:17:UNK:HB2	1.76	0.65
34:FM:218:GLN:HB3	34:FM:243:GLN:HE21	1.62	0.65
12:Cj:195:THR:HG21	15:DD:588:ARG:HE	1.60	0.65
9:Ca:178:PHE:HA	50:UP:1:UNK:HB2	1.78	0.64
34:FM:39:HIS:HB2	34:FM:71:MET:HE3	1.80	0.64
7:CQ:211:ALA:HB2	59:UY:160:UNK:HG1	1.79	0.64
3:CH:111:GLN:HE21	3:CH:113:LYS:HE2	1.63	0.63
59:UY:389:UNK:HB1	59:UY:455:UNK:HB1	1.80	0.63
59:UY:290:UNK:HG2	59:UY:320:UNK:HG2	1.80	0.63
30:FA:19:ARG:HH12	30:FA:544:LYS:HD3	1.63	0.63
59:UY:188:UNK:HB2	59:UY:193:UNK:HB2	1.80	0.63
59:UY:39:UNK:HB1	59:UY:402:UNK:HB1	1.80	0.63
9:Ca:419:GLN:HB2	36:FP:334:THR:HG23	1.79	0.63
59:UY:113:UNK:HB1	59:UY:122:UNK:HB1	1.79	0.63
59:UY:342:UNK:HG2	59:UY:408:UNK:HB1	1.79	0.63
39:FX:109:ARG:HH12	54:UN:8:UNK:HB1	1.65	0.62
59:UY:37:UNK:HB2	59:UY:41:UNK:HG3	1.81	0.62
9:Ca:142:MET:HE3	9:Ca:147:VAL:HG12	1.80	0.62
31:FC:489:GLN:HB2	31:FC:492:GLU:HB3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:UY:352:UNK:HG2	60:CA:542:G:H5''	1.81	0.61
6:CP:188:LEU:HD13	15:DD:226:THR:HG22	1.82	0.61
7:CQ:215:GLN:HG2	59:UY:156:UNK:HG1	1.82	0.61
27:F7:94:ARG:HH22	59:UY:302:UNK:HB1	1.65	0.61
34:FN:90:HIS:HA	34:FN:94:GLU:HB2	1.82	0.61
1:CE:300:ILE:HG22	1:CE:302:PRO:HD2	1.82	0.61
4:CK:280:ARG:HB3	4:CK:310:ILE:HG12	1.82	0.61
36:FP:255:THR:O	36:FP:255:THR:OG1	2.17	0.61
4:CK:310:ILE:HG22	40:FY:141:SER:HB3	1.83	0.61
5:CO:429:ASN:HD21	7:CQ:158:HIS:HE1	1.49	0.61
15:DD:45:GLN:NE2	15:DD:48:MET:SD	2.73	0.61
18:DO:157:ILE:HD12	18:DO:188:ALA:HB1	1.82	0.61
59:UY:140:UNK:HG2	59:UY:143:UNK:HB1	1.83	0.61
3:CH:36:GLY:O	3:CH:53:ARG:NH2	2.33	0.60
11:Cd:171:LYS:HG3	11:Cd:173:GLU:H	1.64	0.60
59:UY:274:UNK:HG3	59:UY:292:UNK:HB1	1.83	0.60
9:Ca:283:PRO:HG2	23:F2:626:MET:HE1	1.81	0.60
26:F6:416:ASP:HB3	26:F6:452:VAL:HG23	1.82	0.60
11:Cd:70:ARG:HH11	15:DD:156:GLN:HE21	1.48	0.60
20:DR:41:HIS:HD1	20:DR:110:TYR:HH	1.49	0.60
34:FM:140:SER:HB3	34:FM:152:LEU:HB3	1.83	0.60
59:UY:254:UNK:HB2	59:UY:437:UNK:HG3	1.84	0.60
27:F7:121:ARG:HH21	27:F7:143:LEU:HD22	1.65	0.60
46:UA:18:UNK:HB1	57:UO:17:UNK:HA	1.84	0.60
24:F3:774:ASP:H	24:F3:812:LEU:HD11	1.67	0.59
27:F7:204:ILE:HB	59:UY:277:UNK:HB2	1.84	0.59
30:FA:417:ILE:HG22	30:FA:419:CYS:H	1.67	0.59
12:Cj:10:ARG:NH1	60:CA:76:A:OP1	2.36	0.59
24:F3:395:LEU:HD12	24:F3:505:LEU:HD22	1.84	0.59
24:F3:352:PHE:H	24:F3:405:ASN:HD21	1.50	0.59
35:FO:147:ASN:HD21	35:FO:180:ARG:HD2	1.67	0.59
60:CA:26:C:H42	60:CA:268:U:H4'	1.68	0.59
8:CR:206:GLU:HA	57:UO:3:UNK:HG3	1.85	0.59
9:Ca:296:THR:HG22	9:Ca:299:ARG:HH11	1.68	0.59
37:FT:34:THR:HG22	37:FT:36:PHE:H	1.67	0.59
59:UY:62:UNK:HB2	59:UY:64:UNK:HG3	1.84	0.59
16:DI:391:ASP:OD1	16:DI:391:ASP:N	2.35	0.59
23:F2:627:LYS:HE3	23:F2:708:GLY:HA3	1.83	0.59
24:F3:386:VAL:HG13	24:F3:390:GLU:HB2	1.85	0.59
28:F8:495:TYR:HB2	28:F8:684:LEU:HB2	1.85	0.59
9:Ca:73:GLU:HB2	9:Ca:79:MET:HG2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:CH:41:VAL:HA	5:CO:115:GLN:HE21	1.68	0.59
6:CP:29:ILE:HG12	6:CP:47:VAL:HG22	1.85	0.58
30:FA:90:CYS:SG	30:FA:91:GLY:N	2.76	0.58
11:Cd:20:SER:HB3	11:Cd:29:THR:HG23	1.84	0.58
30:FA:513:LEU:HD23	30:FA:545:LYS:HB3	1.85	0.58
34:FM:90:HIS:HA	34:FM:94:GLU:HB2	1.85	0.58
9:Ca:134:LEU:HD22	41:FZ:58:LEU:HD11	1.85	0.58
59:UY:90:UNK:HG1	59:UY:139:UNK:HG3	1.84	0.58
16:DI:186:ILE:HG12	16:DI:197:VAL:HG22	1.86	0.58
27:F7:155:LEU:HD13	27:F7:202:THR:HG21	1.85	0.58
1:CE:235:ASN:ND2	60:CA:26:C:OP1	2.36	0.58
35:FO:135:ASN:ND2	37:FQ:176:TYR:OH	2.37	0.58
37:FR:36:PHE:HB2	37:FR:96:TRP:HB3	1.84	0.58
28:F8:234:ARG:HD2	28:F8:238:ARG:HH21	1.67	0.58
30:FA:164:THR:HG23	30:FA:167:ALA:H	1.68	0.58
32:FE:284:ASP:N	32:FE:284:ASP:OD1	2.37	0.58
45:Fd:75:GLY:HA2	45:Fd:96:GLU:HB3	1.86	0.58
16:DI:233:ARG:NH2	16:DI:270:ASP:OD1	2.37	0.58
31:FC:537:PRO:HG3	31:FC:542:PHE:HB3	1.84	0.58
28:F8:507:HIS:HB2	28:F8:609:LYS:HB2	1.86	0.58
29:F9:53:GLU:O	29:F9:109:ARG:NH2	2.37	0.58
34:FN:24:ARG:HA	34:FN:53:LEU:HD21	1.85	0.58
25:F5:641:ARG:HB3	43:Fb:111:VAL:HG13	1.85	0.57
39:FX:115:LYS:HD3	54:UN:2:UNK:HB2	1.87	0.57
7:CQ:93:ASP:HB3	7:CQ:146:HIS:HE1	1.68	0.57
12:Cj:205:ARG:NH2	20:DR:232:THR:O	2.36	0.57
21:DU:106:PRO:HG2	21:DU:109:SER:HB3	1.86	0.57
16:DI:307:ASN:HB3	16:DI:310:LEU:HB2	1.86	0.57
19:DP:64:MET:HA	24:F3:472:GLU:HG2	1.85	0.57
15:DD:709:ARG:NH2	60:CA:138:U:OP1	2.38	0.57
34:FM:302:MET:SD	34:FM:305:ARG:NH1	2.77	0.57
27:F7:121:ARG:HE	27:F7:143:LEU:HD13	1.69	0.57
31:FB:379:THR:HB	37:FT:140:GLY:HA3	1.87	0.57
33:FJ:206:VAL:HG22	33:FJ:217:ILE:HG22	1.87	0.57
36:FP:45:ALA:HB1	36:FP:298:VAL:HG13	1.86	0.57
7:CQ:151:ARG:NH2	20:DR:13:PHE:O	2.38	0.57
28:F8:564:SER:HB3	32:FE:47:SER:HB2	1.87	0.57
31:FB:487:VAL:HG21	37:FU:278:MET:HB2	1.87	0.57
2:CF:86:HIS:HD2	2:CF:88:ASP:H	1.53	0.57
9:Ca:201:ARG:NH1	22:DZ:87:ILE:O	2.38	0.56
27:F7:424:LEU:HD11	27:F7:624:PRO:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:FU:131:VAL:HB	37:FU:242:HIS:HB2	1.86	0.56
24:F3:169:ARG:NH2	60:CA:104:A:O2'	2.37	0.56
27:F7:203:ASN:HB3	59:UY:278:UNK:HG1	1.86	0.56
37:FQ:146:LEU:HB3	37:FQ:189:PHE:HB3	1.87	0.56
59:UY:186:UNK:HG2	59:UY:195:UNK:HG2	1.88	0.56
31:FC:483:ARG:HB3	31:FC:498:VAL:HB	1.86	0.56
59:UY:192:UNK:O	59:UY:278:UNK:HB1	2.05	0.56
5:CO:215:ASP:OD2	11:Cd:124:ARG:NH1	2.39	0.56
4:CK:191:ASP:OD2	4:CK:267:ARG:NH1	2.38	0.56
16:DI:342:ARG:NH2	16:DI:400:ASN:O	2.39	0.56
31:FC:188:ARG:NH1	31:FC:284:CYS:SG	2.79	0.56
32:FE:76:GLN:HG2	32:FE:90:LEU:HD21	1.88	0.56
42:Fa:24:TYR:HB2	42:Fa:27:VAL:HG22	1.88	0.56
49:UD:7:UNK:HG3	51:UF:9:UNK:HB2	1.88	0.56
9:Ca:350:GLU:HG3	15:DD:107:ASP:HA	1.88	0.56
24:F3:884:MET:O	24:F3:892:ARG:NH2	2.38	0.56
27:F7:203:ASN:HB3	59:UY:278:UNK:CG	2.36	0.56
28:F8:595:ARG:NH1	32:FE:78:GLU:O	2.39	0.56
59:UY:291:UNK:HB1	59:UY:319:UNK:HG2	1.86	0.56
6:CP:136:PRO:HD2	38:FW:137:PRO:HB2	1.88	0.56
31:FB:275:GLU:OE2	31:FB:508:ARG:NH1	2.35	0.56
37:FU:134:HIS:HB2	37:FU:145:ALA:HB3	1.87	0.56
2:CF:52:ARG:NH2	40:FY:132:ASP:OD2	2.39	0.56
16:DI:340:ARG:HB3	16:DI:404:TRP:HB3	1.88	0.56
28:F8:53:ARG:HB2	28:F8:82:ARG:HH11	1.71	0.56
25:F5:447:VAL:HA	25:F5:450:MET:HE2	1.87	0.55
33:FJ:30:VAL:HG13	60:CA:615:U:H1'	1.87	0.55
16:DI:326:ARG:NH1	18:DO:201:GLU:OE2	2.38	0.55
24:F3:173:ARG:NH2	60:CA:116:U:O2	2.39	0.55
31:FB:329:HIS:HD2	31:FB:331:ARG:H	1.55	0.55
17:DL:84:GLU:OE2	17:DL:209:ARG:NH1	2.40	0.55
30:FA:275:LEU:O	30:FA:353:LYS:NZ	2.37	0.55
30:FA:162:CYS:HB3	30:FA:171:ALA:HB2	1.88	0.55
30:FA:561:ASN:ND2	30:FA:632:GLU:OE2	2.40	0.55
31:FB:476:PRO:O	31:FB:479:ARG:NH1	2.40	0.55
59:UY:287:UNK:HA	59:UY:323:UNK:HA	1.87	0.55
3:CH:98:ARG:HH22	16:DI:308:PRO:HG3	1.72	0.55
31:FB:361:ASP:O	31:FC:298:ARG:NH1	2.39	0.55
16:DI:18:HIS:HD2	16:DI:65:MET:HB2	1.70	0.55
5:CO:264:ARG:NH1	5:CO:300:TYR:O	2.39	0.55
15:DD:709:ARG:HE	60:CA:138:U:H5'	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:FO:6:ARG:HB3	59:UY:155:UNK:HG2	1.88	0.55
37:FT:146:LEU:HB3	37:FT:189:PHE:HB3	1.89	0.55
42:Fa:30:THR:HG22	42:Fa:80:PRO:HB3	1.88	0.55
15:DD:608:ASP:OD1	20:DR:221:ARG:NH2	2.40	0.55
19:DP:79:ARG:O	35:FO:248:ARG:NH1	2.40	0.55
31:FC:503:LEU:HD23	52:UG:10:UNK:HB1	1.89	0.55
37:FR:144:HIS:HB2	37:FR:191:THR:HB	1.87	0.55
38:FW:60:ILE:HD11	38:FW:257:LEU:HD21	1.88	0.55
52:UG:10:UNK:HG3	52:UG:14:UNK:HB1	1.88	0.55
3:CH:48:ASP:OD1	3:CH:201:ARG:NH1	2.40	0.55
15:DD:325:LYS:O	15:DD:385:ASN:ND2	2.40	0.55
24:F3:418:ASP:OD1	24:F3:418:ASP:N	2.36	0.55
31:FB:504:ARG:NH1	60:CA:243:C:OP2	2.40	0.55
35:FO:162:GLU:OE1	35:FO:164:ARG:NH1	2.40	0.55
37:FU:227:THR:HB	37:FU:241:ILE:HB	1.88	0.55
30:FA:183:LEU:HD11	47:UB:1:UNK:HG2	1.89	0.54
7:CQ:144:LEU:HB3	7:CQ:166:GLU:HB3	1.89	0.54
30:FA:549:PRO:HA	30:FA:552:LEU:HB2	1.89	0.54
37:FT:131:VAL:HB	37:FT:242:HIS:HB3	1.90	0.54
1:CE:91:ASN:O	1:CE:120:ASN:ND2	2.39	0.54
15:DD:77:SER:O	15:DD:85:ASN:ND2	2.41	0.54
32:FE:270:ARG:NH1	60:CA:36:U:OP2	2.40	0.54
36:FP:26:ASP:OD2	36:FP:30:ARG:NH1	2.40	0.54
44:Fc:96:HIS:HD2	44:Fc:99:ASN:H	1.54	0.54
1:CE:154:PHE:HD1	33:FJ:75:LEU:HD13	1.73	0.54
9:Ca:106:ASN:HB2	9:Ca:155:ARG:HD3	1.88	0.54
15:DD:44:MET:SD	15:DD:57:HIS:NE2	2.79	0.54
16:DI:83:GLN:HE21	16:DI:175:GLN:HE21	1.53	0.54
26:F6:374:TRP:HZ3	56:UL:19:UNK:HG1	1.72	0.54
31:FC:256:ALA:HB2	31:FC:308:MET:HE3	1.88	0.54
36:FP:156:TRP:O	39:FX:42:ARG:NH2	2.39	0.54
7:CQ:194:ARG:NH2	7:CQ:220:ASP:OD2	2.41	0.54
19:DP:183:ASP:OD1	19:DP:183:ASP:N	2.36	0.54
22:DZ:69:HIS:HB3	22:DZ:72:LEU:HD23	1.87	0.54
26:F6:329:LEU:HD22	26:F6:336:LEU:HD11	1.88	0.54
34:FN:237:ARG:HG2	38:FW:2:SER:HB3	1.90	0.54
35:FO:220:VAL:HG11	35:FO:240:SER:HB3	1.89	0.54
37:FS:11:ARG:HD2	37:FS:22:GLU:HB3	1.90	0.54
10:Cb:95:ARG:NH1	10:Cb:126:GLU:OE2	2.41	0.54
26:F6:220:LEU:HB2	57:UO:12:UNK:HA	1.89	0.54
60:CA:77:A:H3'	60:CA:78:G:H2'	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:CR:64:VAL:HG11	10:Cb:179:GLU:HG3	1.90	0.54
33:FJ:135:ARG:NH2	42:Fa:127:LYS:O	2.40	0.54
34:FM:13:VAL:HA	34:FM:39:HIS:HB3	1.89	0.54
2:CF:100:ARG:NH2	60:CA:309:A:OP2	2.41	0.54
24:F3:520:SER:HA	24:F3:558:MET:HE3	1.89	0.54
30:FA:565:PRO:HB3	30:FA:593:LEU:HD22	1.89	0.54
35:FO:292:ARG:NH1	35:FO:298:TRP:O	2.39	0.54
22:DZ:80:TRP:HB3	22:DZ:87:ILE:HD12	1.89	0.54
34:FM:196:VAL:HG13	34:FM:234:MET:HE3	1.90	0.54
36:FP:44:ALA:HB1	36:FP:75:VAL:HG13	1.90	0.54
36:FP:46:ARG:O	36:FP:46:ARG:NH1	2.40	0.54
7:CQ:211:ALA:HB2	59:UY:160:UNK:CG	2.38	0.54
9:Ca:160:GLU:OE1	9:Ca:223:ASN:ND2	2.41	0.54
15:DD:238:GLU:OE1	16:DI:18:HIS:N	2.41	0.54
25:F5:351:ARG:NH2	25:F5:464:GLU:OE1	2.41	0.54
25:F5:733:PRO:HB2	25:F5:744:ARG:HG2	1.90	0.54
32:FE:248:ARG:HH21	32:FE:277:ARG:HG3	1.72	0.54
35:FO:183:ARG:HH11	49:UM:8:UNK:HB2	1.72	0.54
35:FO:296:GLN:HA	51:UF:6:UNK:HG1	1.90	0.54
37:FQ:71:LEU:HD21	37:FQ:98:LEU:HD21	1.89	0.54
37:FS:133:ASP:HB3	37:FS:240:LEU:HB3	1.89	0.54
3:CH:195:ARG:HB2	3:CH:204:ALA:HB3	1.90	0.53
18:DO:172:ALA:HB2	27:F7:564:LEU:HD13	1.90	0.53
25:F5:648:PRO:HG2	43:Fb:96:VAL:HG12	1.90	0.53
31:FB:441:ASN:HB2	32:FE:148:GLU:HB2	1.90	0.53
37:FT:228:LEU:HD11	37:FT:238:ARG:HB3	1.90	0.53
59:UY:140:UNK:HB2	59:UY:142:UNK:HG3	1.90	0.53
25:F5:327:ARG:HD3	25:F5:490:ASP:HA	1.89	0.53
27:F7:208:GLU:HG2	59:UY:188:UNK:HB1	1.89	0.53
32:FE:193:PHE:O	32:FE:255:ARG:NH2	2.41	0.53
4:CK:319:LYS:O	40:FY:184:ARG:NH2	2.42	0.53
11:Cd:11:GLN:HB3	60:CA:48:U:H4'	1.90	0.53
37:FQ:36:PHE:HB2	37:FQ:96:TRP:HB3	1.90	0.53
37:FR:90:VAL:O	37:FR:94:ASN:ND2	2.35	0.53
37:FR:139:GLN:NE2	60:CA:562:U:O2	2.42	0.53
37:FR:235:THR:HG21	37:FS:238:ARG:HH21	1.73	0.53
24:F3:92:ARG:NH1	24:F3:93:GLU:O	2.41	0.53
24:F3:532:LEU:HD13	24:F3:551:LEU:HD11	1.91	0.53
35:FO:183:ARG:NH1	49:UM:8:UNK:HB2	2.22	0.53
60:CA:248:A:H2'	60:CA:249:U:C6	2.44	0.53
14:Cp:12:THR:O	14:Cp:17:LYS:NZ	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Cp:66:HIS:HD2	14:Cp:68:LEU:H	1.56	0.53
59:UY:256:UNK:HG2	59:UY:321:UNK:HB1	1.89	0.53
9:Ca:531:ASP:OD1	15:DD:202:ARG:NH1	2.42	0.53
38:FW:34:ILE:HD11	38:FW:251:LEU:HD22	1.91	0.53
1:CE:361:ASN:HA	16:DI:122:ASN:HD21	1.74	0.53
8:CR:186:ARG:NH1	26:F6:442:ALA:O	2.38	0.53
12:Cj:155:GLU:OE1	15:DD:626:ARG:NH2	2.40	0.53
24:F3:103:ASP:O	24:F3:175:ARG:NH1	2.41	0.53
31:FC:190:ASP:OD2	31:FC:319:SER:OG	2.27	0.53
59:UY:153:UNK:CB	59:UY:299:UNK:HG1	2.38	0.53
5:CO:121:GLY:O	11:Cd:130:GLN:NE2	2.38	0.53
9:Ca:420:GLN:HA	9:Ca:481:ARG:HA	1.89	0.53
10:Cb:183:VAL:HA	10:Cb:186:VAL:HG12	1.91	0.53
24:F3:728:ARG:HG2	24:F3:777:ARG:HD3	1.91	0.53
35:FO:101:ARG:NH2	35:FO:102:ILE:O	2.42	0.53
60:CA:271:A:N6	60:CA:371:U:OP1	2.40	0.53
3:CH:210:PHE:HB2	23:F2:337:GLN:HE21	1.72	0.53
9:Ca:89:ARG:HH11	50:UP:3:UNK:HB1	1.74	0.53
30:FA:248:SER:O	30:FA:252:HIS:ND1	2.41	0.53
23:F2:352:ARG:NH1	23:F2:387:VAL:O	2.42	0.53
31:FC:193:TYR:HB3	31:FC:315:LEU:HD12	1.92	0.53
37:FQ:238:ARG:NH1	37:FT:229:SER:OG	2.42	0.53
28:F8:494:THR:HB	28:F8:604:VAL:HB	1.90	0.52
34:FN:37:GLN:HG2	34:FN:63:ARG:HB2	1.89	0.52
33:FJ:286:ALA:O	33:FJ:290:LEU:HB2	2.09	0.52
59:UY:172:UNK:HG3	59:UY:232:UNK:HG1	1.92	0.52
37:FQ:136:GLN:HG2	37:FQ:237:VAL:HG22	1.91	0.52
37:FR:74:ASN:OD1	37:FR:251:ARG:NH2	2.42	0.52
6:CP:45:LEU:HD21	6:CP:117:LEU:HD23	1.90	0.52
15:DD:181:MET:HE1	15:DD:215:TYR:HD1	1.74	0.52
24:F3:244:LEU:HB3	27:F7:63:ARG:HH21	1.75	0.52
32:FE:355:VAL:HG21	32:FE:393:LEU:HD21	1.90	0.52
37:FQ:146:LEU:HD21	37:FQ:206:VAL:HG11	1.91	0.52
3:CH:209:TYR:O	23:F2:337:GLN:NE2	2.43	0.52
26:F6:131:ARG:HA	26:F6:134:LEU:HB2	1.92	0.52
29:F9:144:ASP:OD2	29:F9:147:ARG:NH2	2.42	0.52
33:FJ:104:GLY:HA3	33:FJ:127:ILE:H	1.74	0.52
35:FO:292:ARG:HB3	35:FO:306:ASN:HB3	1.91	0.52
37:FS:63:VAL:HG22	37:FS:85:ILE:HG23	1.92	0.52
16:DI:148:ALA:O	16:DI:152:LEU:HB2	2.09	0.52
28:F8:527:GLN:HB3	28:F8:546:PHE:HE2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:DD:303:LEU:HD21	15:DD:400:VAL:HG23	1.92	0.52
16:DI:233:ARG:NH2	16:DI:272:CYS:O	2.43	0.52
2:CF:159:ARG:HH21	26:F6:314:LEU:HB3	1.75	0.52
3:CH:93:GLY:HA2	3:CH:111:GLN:O	2.10	0.52
26:F6:45:PHE:HD2	26:F6:122:VAL:HG11	1.75	0.52
34:FN:72:THR:O	34:FN:104:ARG:NH1	2.42	0.52
59:UY:125:UNK:HA	59:UY:127:UNK:HG2	1.92	0.52
5:CO:215:ASP:OD1	5:CO:215:ASP:N	2.41	0.52
5:CO:413:LEU:HD22	5:CO:417:LYS:HD2	1.92	0.52
7:CQ:224:PHE:HA	27:F7:87:PRO:HG2	1.92	0.52
14:Cp:139:SER:OG	14:Cp:141:ARG:NE	2.43	0.52
18:DO:68:ARG:NH1	18:DO:72:GLU:OE2	2.43	0.52
23:F2:855:SER:O	25:F5:468:ARG:NH1	2.43	0.52
29:F9:59:VAL:HG11	29:F9:116:ASP:HB2	1.91	0.52
34:FN:70:THR:O	34:FN:74:TRP:HB2	2.10	0.52
16:DI:385:LEU:HD13	16:DI:393:THR:HG22	1.92	0.51
21:DU:86:ILE:HD13	21:DU:99:GLN:HB2	1.93	0.51
35:FO:25:TRP:HH2	49:UD:5:UNK:O	1.92	0.51
37:FS:136:GLN:HB2	37:FS:143:ARG:HB3	1.92	0.51
43:Fb:77:LEU:HB3	65:FcA:1:PM8:H21	1.92	0.51
7:CQ:70:ARG:NE	60:CA:149:U:OP2	2.43	0.51
15:DD:597:LEU:HD13	15:DD:620:ALA:HB1	1.93	0.51
16:DI:290:PHE:HB2	16:DI:301:ILE:HB	1.92	0.51
27:F7:614:ASP:OD2	53:UH:1:UNK:N	2.43	0.51
37:FR:129:VAL:HB	37:FR:244:PHE:HB2	1.92	0.51
40:FY:156:ARG:HH21	40:FY:180:THR:HG23	1.75	0.51
50:UE:9:UNK:O	50:UE:13:UNK:N	2.44	0.51
5:CO:210:ARG:NH2	5:CO:276:GLU:OE2	2.43	0.51
7:CQ:67:LEU:HG	15:DD:709:ARG:HH22	1.75	0.51
33:FJ:74:ARG:HA	33:FJ:77:ARG:HD2	1.93	0.51
6:CP:19:GLN:NE2	60:CA:174:A:O2'	2.43	0.51
19:DP:27:ASP:N	19:DP:27:ASP:OD1	2.44	0.51
34:FN:302:MET:SD	34:FN:305:ARG:NH1	2.83	0.51
37:FS:93:MET:HG2	37:FS:98:LEU:HB3	1.92	0.51
37:FS:269:ILE:HB	62:FF:4:ILE:HG12	1.90	0.51
3:CH:24:GLY:O	27:F7:450:ASN:ND2	2.43	0.51
7:CQ:47:LYS:HB2	7:CQ:50:ALA:HB3	1.90	0.51
9:Ca:443:MET:HE1	9:Ca:487:GLU:HB3	1.93	0.51
23:F2:245:ARG:NH1	60:CA:2:A:O2'	2.44	0.51
28:F8:496:LEU:HB2	28:F8:602:VAL:HB	1.91	0.51
35:FO:130:THR:HG23	35:FO:133:MET:HE3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:FW:18:ARG:NH1	38:FW:206:MET:O	2.44	0.51
7:CQ:30:ARG:NH1	60:CA:153:A:OP2	2.44	0.51
9:Ca:363:ARG:NH2	23:F2:596:GLU:OE1	2.43	0.51
16:DI:282:ASP:O	16:DI:313:ARG:NH1	2.44	0.51
18:DO:193:LEU:HD12	18:DO:234:LEU:HD22	1.93	0.51
25:F5:722:GLU:HA	25:F5:725:ARG:HG2	1.92	0.51
31:FB:490:ASP:HB3	31:FC:282:ARG:HH22	1.75	0.51
33:FJ:51:ARG:NH1	33:FJ:90:GLY:O	2.44	0.51
39:FX:211:HIS:HB2	39:FX:213:TRP:HD1	1.76	0.51
14:Cp:149:LYS:HD2	28:F8:44:MET:HG2	1.93	0.51
27:F7:269:VAL:HG11	27:F7:301:LEU:HB2	1.92	0.51
28:F8:537:HIS:NE2	37:FT:182:THR:O	2.43	0.51
29:F9:81:ARG:NH1	29:F9:96:GLU:OE2	2.43	0.51
31:FB:361:ASP:OD1	31:FB:361:ASP:N	2.43	0.51
31:FC:572:GLN:HG2	31:FC:573:PHE:HD1	1.76	0.51
41:FZ:52:ILE:HA	41:FZ:56:ILE:HD12	1.92	0.51
59:UY:53:UNK:HB1	59:UY:397:UNK:HG3	1.92	0.51
7:CQ:134:ASP:N	7:CQ:134:ASP:OD1	2.42	0.51
7:CQ:166:GLU:OE1	15:DD:261:ARG:NH1	2.44	0.51
35:FO:6:ARG:NH1	59:UY:386:UNK:HG2	2.25	0.51
37:FR:134:HIS:HB2	37:FR:145:ALA:HB3	1.92	0.51
9:Ca:232:GLN:O	9:Ca:238:GLN:NE2	2.44	0.51
10:Cb:131:GLU:OE2	10:Cb:134:ARG:NH2	2.44	0.51
30:FA:56:VAL:HG12	30:FA:76:LEU:HD21	1.92	0.51
30:FA:242:SER:HB3	47:UB:206:UNK:HG1	1.93	0.51
37:FQ:94:ASN:HA	37:FQ:99:LEU:HD22	1.92	0.51
37:FR:78:LEU:HB3	37:FR:86:ARG:HG3	1.93	0.51
3:CH:194:PHE:HB2	23:F2:304:MET:HG2	1.91	0.50
7:CQ:153:ILE:O	20:DR:10:SER:N	2.44	0.50
15:DD:95:ARG:NH1	60:CA:143:U:O4	2.45	0.50
15:DD:157:GLU:HA	15:DD:160:HIS:HB3	1.93	0.50
15:DD:250:LYS:O	15:DD:287:ARG:NE	2.44	0.50
27:F7:279:VAL:HG21	27:F7:290:MET:HE1	1.93	0.50
29:F9:194:MET:HE1	41:FZ:165:ALA:HB3	1.92	0.50
34:FM:255:THR:HA	34:FM:305:ARG:HA	1.93	0.50
50:UE:10:UNK:HA	50:UE:13:UNK:HB2	1.92	0.50
59:UY:284:UNK:HB2	59:UY:329:UNK:HG1	1.93	0.50
8:CR:79:ASN:OD1	8:CR:82:ARG:NH1	2.44	0.50
10:Cb:133:LYS:NZ	10:Cb:138:ASP:O	2.44	0.50
11:Cd:51:GLU:OE2	12:Cj:15:ASN:ND2	2.44	0.50
14:Cp:122:ASP:OD1	14:Cp:124:LYS:NZ	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:FO:148:ARG:HH21	54:UI:2:UNK:HB1	1.76	0.50
60:CA:241:U:O2'	60:CA:242:G:O4'	2.28	0.50
20:DR:64:ILE:HD11	20:DR:154:LEU:HD23	1.94	0.50
23:F2:14:PRO:HA	23:F2:17:GLN:HB2	1.93	0.50
31:FC:491:ASP:OD1	31:FC:491:ASP:N	2.44	0.50
32:FE:300:ILE:HB	32:FE:348:ILE:HG22	1.92	0.50
32:FE:314:THR:HG22	32:FE:326:GLY:HA3	1.93	0.50
59:UY:202:UNK:HA	59:UY:205:UNK:HG3	1.93	0.50
5:CO:149:GLN:O	11:Cd:143:GLN:NE2	2.44	0.50
6:CP:39:LYS:HB3	38:FW:172:THR:HG21	1.94	0.50
9:Ca:89:ARG:HA	50:UP:5:UNK:HG2	1.93	0.50
9:Ca:244:PRO:HA	9:Ca:247:PHE:HB2	1.93	0.50
15:DD:387:GLN:HE22	15:DD:453:ASN:H	1.58	0.50
16:DI:367:SER:H	16:DI:370:GLN:HE21	1.58	0.50
18:DO:86:ARG:NH2	18:DO:126:PRO:O	2.43	0.50
27:F7:295:MET:O	27:F7:299:SER:OG	2.29	0.50
34:FN:196:VAL:HG13	34:FN:234:MET:HE3	1.94	0.50
7:CQ:106:THR:HA	7:CQ:132:ALA:O	2.12	0.50
24:F3:545:LEU:HD11	24:F3:598:LEU:HD22	1.94	0.50
31:FC:489:GLN:NE2	37:FU:282:PRO:O	2.44	0.50
37:FU:143:ARG:NH1	60:CA:240:U:O4	2.44	0.50
39:FX:125:LYS:NZ	39:FX:157:ASP:O	2.44	0.50
5:CO:159:LYS:NZ	27:F7:494:ASP:OD2	2.39	0.50
8:CR:177:PRO:O	8:CR:181:ARG:NH2	2.45	0.50
23:F2:637:ARG:NH1	23:F2:698:HIS:O	2.44	0.50
30:FA:414:PRO:HB2	30:FA:449:SER:HB3	1.93	0.50
15:DD:410:THR:HG22	15:DD:417:THR:HG21	1.93	0.50
23:F2:205:THR:OG1	23:F2:206:GLU:N	2.45	0.50
23:F2:617:ASN:OD1	23:F2:624:ARG:NH2	2.44	0.50
24:F3:159:ASN:OD1	27:F7:101:ARG:NH2	2.45	0.50
24:F3:689:CYS:O	24:F3:714:TYR:OH	2.30	0.50
31:FC:186:ARG:NH1	31:FC:328:PHE:O	2.45	0.50
31:FC:303:ARG:NH2	32:FE:374:ASN:O	2.45	0.50
35:FO:295:ARG:NE	35:FO:331:PHE:O	2.44	0.50
7:CQ:20:GLN:HE22	21:DU:219:THR:H	1.59	0.50
12:Cj:72:ASP:OD1	12:Cj:72:ASP:N	2.41	0.50
14:Cp:41:ILE:HG22	14:Cp:42:VAL:HG23	1.94	0.50
23:F2:729:SER:O	23:F2:732:GLN:NE2	2.45	0.50
28:F8:439:ARG:HH11	28:F8:440:PRO:HD2	1.76	0.50
32:FE:16:ILE:N	32:FE:157:HIS:O	2.45	0.50
16:DI:188:GLU:HG2	16:DI:195:ILE:HG13	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:DI:256:ARG:HB2	16:DI:270:ASP:HB3	1.94	0.50
20:DR:74:GLU:HG2	24:F3:429:LYS:HG3	1.94	0.50
37:FU:19:ARG:NH1	37:FU:65:GLU:OE2	2.45	0.50
39:FX:155:ASP:OD2	39:FX:188:ARG:NH1	2.45	0.50
46:UA:14:UNK:HA	46:UA:17:UNK:HG3	1.93	0.50
60:CA:100:G:O2'	60:CA:127:G:N2	2.41	0.50
10:Cb:86:THR:OG1	10:Cb:87:LEU:N	2.44	0.49
23:F2:297:GLN:O	23:F2:301:ASN:ND2	2.42	0.49
31:FB:205:THR:O	60:CA:244:G:O2'	2.29	0.49
32:FE:159:THR:HB	32:FE:162:GLU:HG3	1.93	0.49
33:FJ:69:TYR:O	33:FJ:74:ARG:NH2	2.45	0.49
38:FW:39:GLY:HA3	38:FW:70:LEU:HG	1.93	0.49
39:FX:37:ALA:O	39:FX:67:ARG:NH2	2.45	0.49
60:CA:245:G:H3'	60:CA:246:U:H2'	1.94	0.49
9:Ca:354:THR:HB	60:CA:19:U:H5''	1.94	0.49
18:DO:97:TYR:HB3	18:DO:109:VAL:HG11	1.93	0.49
23:F2:99:GLY:HA3	23:F2:224:ILE:HG23	1.93	0.49
30:FA:41:ASP:OD1	30:FA:41:ASP:N	2.45	0.49
33:FJ:320:LYS:NZ	60:CA:375:A:OP1	2.45	0.49
44:Fc:78:GLU:O	44:Fc:82:ASN:ND2	2.42	0.49
59:UY:55:UNK:HB1	59:UY:395:UNK:HG1	1.93	0.49
21:DU:146:THR:OG1	24:F3:518:ARG:NH1	2.45	0.49
23:F2:933:LYS:NZ	29:F9:53:GLU:OE2	2.39	0.49
29:F9:47:ARG:HA	29:F9:50:GLU:HG2	1.95	0.49
31:FB:450:THR:OG1	32:FE:141:ARG:NH1	2.44	0.49
59:UY:227:UNK:HA	59:UY:230:UNK:HG3	1.95	0.49
1:CE:302:PRO:HG2	23:F2:607:PRO:HG3	1.94	0.49
7:CQ:72:ARG:NH2	60:CA:149:U:O4	2.46	0.49
24:F3:169:ARG:NH2	60:CA:106:U:O2	2.46	0.49
27:F7:304:GLN:O	27:F7:308:HIS:ND1	2.45	0.49
59:UY:360:UNK:HA	59:UY:363:UNK:HG3	1.95	0.49
8:CR:212:TRP:NE1	26:F6:458:ASP:OD2	2.46	0.49
21:DU:185:ALA:HB3	21:DU:188:VAL:HB	1.94	0.49
24:F3:765:GLU:OE2	24:F3:768:ARG:NH1	2.46	0.49
34:FM:70:THR:HA	34:FM:73:LYS:HG2	1.94	0.49
37:FQ:14:ILE:HD11	37:FQ:57:LEU:HG	1.94	0.49
7:CQ:65:GLY:HA2	60:CA:136:G:H5'	1.94	0.49
23:F2:11:ALA:HB1	23:F2:879:PRO:HG3	1.94	0.49
23:F2:551:GLU:HG2	39:FX:123:LYS:HA	1.94	0.49
25:F5:200:PHE:HB3	25:F5:626:VAL:HG11	1.95	0.49
27:F7:309:GLU:HA	27:F7:312:ARG:HE	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:FA:446:ILE:HG23	30:FA:451:THR:HB	1.94	0.49
37:FQ:204:THR:HB	37:FT:151:GLY:HA2	1.95	0.49
9:Ca:144:ASP:N	9:Ca:144:ASP:OD1	2.45	0.49
15:DD:221:GLU:O	15:DD:406:ARG:NH2	2.43	0.49
20:DR:16:ASN:ND2	21:DU:53:LEU:O	2.46	0.49
25:F5:652:SER:O	43:Fb:48:ARG:NH1	2.45	0.49
26:F6:223:ALA:HB2	57:UO:11:UNK:HG2	1.95	0.49
27:F7:90:GLU:OE1	27:F7:91:LYS:NZ	2.41	0.49
34:FM:150:GLN:HA	34:FM:174:ASP:HB2	1.95	0.49
35:FO:290:ARG:NH1	35:FO:334:ILE:O	2.46	0.49
1:CE:109:LYS:HA	29:F9:192:LEU:HA	1.95	0.49
5:CO:332:ARG:NH1	5:CO:340:ASP:OD2	2.42	0.49
8:CR:219:ARG:NH2	57:UO:30:UNK:O	2.46	0.49
11:Cd:36:ARG:NE	60:CA:178:A:N1	2.59	0.49
23:F2:831:THR:HG23	23:F2:834:GLU:H	1.78	0.49
32:FE:119:ASN:HD22	32:FE:135:SER:HB2	1.78	0.49
32:FE:296:LYS:NZ	32:FE:340:ASP:O	2.44	0.49
35:FO:6:ARG:N	59:UY:152:UNK:O	2.46	0.49
37:FQ:163:ARG:NH2	37:FQ:212:GLU:OE1	2.45	0.49
12:Cj:125:THR:HB	12:Cj:208:ALA:HB2	1.94	0.49
37:FR:126:VAL:HG22	37:FR:247:ARG:HG2	1.94	0.49
7:CQ:58:HIS:NE2	7:CQ:60:ALA:O	2.46	0.49
16:DI:159:ASP:OD1	16:DI:159:ASP:N	2.42	0.49
23:F2:485:ASN:ND2	60:CA:10:G:O6	2.42	0.49
34:FM:6:ARG:NH1	34:FM:9:ASN:OD1	2.46	0.49
35:FO:303:HIS:HB3	35:FO:306:ASN:HB2	1.94	0.49
38:FW:195:ARG:NH2	38:FW:202:GLU:O	2.45	0.49
38:FW:252:LEU:HD22	38:FW:258:LEU:HD11	1.94	0.49
1:CE:150:ARG:NH1	33:FJ:112:LYS:O	2.46	0.48
8:CR:125:ASN:OD1	8:CR:128:ASN:ND2	2.45	0.48
23:F2:451:ASP:OD1	23:F2:742:ARG:NH2	2.44	0.48
24:F3:518:ARG:NH2	24:F3:561:GLU:O	2.46	0.48
25:F5:207:LYS:HG2	41:FZ:70:VAL:HG13	1.95	0.48
26:F6:256:ASP:OD1	26:F6:256:ASP:N	2.46	0.48
30:FA:381:ALA:HA	30:FA:384:ARG:HH21	1.76	0.48
35:FO:66:VAL:HA	49:UD:1:UNK:H2	1.77	0.48
45:Fd:59:HIS:O	45:Fd:63:ASN:ND2	2.43	0.48
4:CK:281:VAL:HG11	4:CK:288:ARG:HG3	1.94	0.48
5:CO:147:GLU:OE2	18:DO:111:ARG:NH2	2.45	0.48
6:CP:145:LEU:HB3	15:DD:656:LEU:HB3	1.95	0.48
9:Ca:326:PHE:HB3	9:Ca:329:GLU:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:DO:94:ILE:HG23	18:DO:99:LEU:HB2	1.94	0.48
23:F2:745:LEU:HD13	23:F2:794:GLU:HG3	1.95	0.48
26:F6:111:ASN:O	26:F6:118:HIS:NE2	2.46	0.48
27:F7:433:ARG:HE	27:F7:467:ASN:HB3	1.78	0.48
31:FC:332:HIS:HB3	31:FC:335:LEU:HB2	1.95	0.48
32:FE:17:THR:HA	32:FE:156:THR:HG22	1.95	0.48
32:FE:342:LEU:HD11	32:FE:348:ILE:HG23	1.95	0.48
34:FM:190:MET:HB3	34:FM:270:LEU:HD13	1.95	0.48
34:FN:36:LEU:O	34:FN:62:MET:HA	2.12	0.48
59:UY:101:UNK:HB2	59:UY:128:UNK:HG3	1.94	0.48
12:Cj:128:LYS:HB2	12:Cj:152:PHE:HD1	1.77	0.48
26:F6:180:LYS:HB2	26:F6:185:GLU:HG2	1.94	0.48
34:FN:70:THR:HA	34:FN:73:LYS:HG2	1.94	0.48
37:FQ:72:ARG:NH1	37:FT:58:ASP:OD1	2.45	0.48
4:CK:258:LEU:HB3	4:CK:269:MET:HE1	1.96	0.48
5:CO:352:ASN:HB2	60:CA:119:A:H4'	1.94	0.48
9:Ca:135:ALA:HB3	9:Ca:138:LYS:HE2	1.95	0.48
12:Cj:52:LEU:HA	12:Cj:96:THR:HG21	1.95	0.48
14:Cp:137:ASP:OD1	14:Cp:137:ASP:N	2.47	0.48
41:FZ:14:CYS:N	41:FZ:17:SER:OG	2.43	0.48
46:UA:9:UNK:O	46:UA:13:UNK:HG2	2.12	0.48
60:CA:338:U:O2'	60:CA:340:U:OP2	2.31	0.48
3:CH:44:ASP:OD2	5:CO:111:GLN:NE2	2.46	0.48
15:DD:229:MET:HG2	16:DI:186:ILE:HG21	1.94	0.48
17:DL:249:LEU:O	17:DL:254:ARG:NH1	2.46	0.48
31:FC:252:VAL:HA	31:FC:255:GLU:HG2	1.95	0.48
34:FN:39:HIS:HB2	34:FN:71:MET:HE3	1.95	0.48
35:FO:214:ARG:HD2	35:FO:242:MET:HG3	1.94	0.48
40:FY:150:ASP:OD1	40:FY:150:ASP:N	2.45	0.48
3:CH:199:ASN:ND2	3:CH:202:ALA:O	2.45	0.48
7:CQ:88:PRO:HB3	15:DD:129:ARG:HA	1.95	0.48
14:Cp:30:LEU:O	34:FM:31:ARG:NH1	2.45	0.48
15:DD:605:ARG:O	20:DR:227:ARG:NH2	2.47	0.48
23:F2:536:TYR:HE1	23:F2:555:LEU:HD12	1.77	0.48
25:F5:343:LEU:HD23	25:F5:468:ARG:HH11	1.78	0.48
29:F9:202:LYS:HE2	29:F9:210:GLN:HA	1.95	0.48
29:F9:216:LEU:HD21	41:FZ:165:ALA:HB2	1.96	0.48
50:UE:12:UNK:HA	50:UE:15:UNK:HB2	1.95	0.48
59:UY:77:UNK:O	59:UY:81:UNK:HG3	2.13	0.48
2:CF:53:ASP:O	45:Fd:29:ASN:ND2	2.46	0.48
30:FA:606:SER:O	30:FA:610:HIS:ND1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:CP:123:LEU:O	11:Cd:61:TYR:OH	2.30	0.48
23:F2:178:ALA:HB2	23:F2:235:MET:HB3	1.96	0.48
26:F6:430:TRP:HE1	26:F6:468:LEU:HB2	1.78	0.48
31:FB:339:TYR:HB3	31:FB:555:LEU:HD11	1.94	0.48
31:FB:500:ARG:NH1	60:CA:240:U:O2'	2.47	0.48
32:FE:388:ARG:HH21	61:F1:1010:ALA:HB1	1.78	0.48
5:CO:313:THR:O	15:DD:261:ARG:NH2	2.44	0.48
9:Ca:78:PHE:HE2	9:Ca:176:ILE:HG22	1.77	0.48
12:Cj:159:ARG:NH1	15:DD:353:HIS:O	2.40	0.48
14:Cp:17:LYS:HE2	23:F2:766:GLY:HA3	1.95	0.48
20:DR:126:LEU:HB2	20:DR:135:CYS:HB3	1.96	0.48
27:F7:10:ARG:N	27:F7:334:GLU:OE2	2.47	0.48
35:FO:154:LEU:HB3	54:UI:8:UNK:HG2	1.95	0.48
1:CE:60:TYR:HE1	1:CE:244:ALA:HB2	1.79	0.48
15:DD:571:VAL:HG22	15:DD:603:GLU:HB2	1.96	0.48
24:F3:332:VAL:HG11	24:F3:390:GLU:HB3	1.95	0.48
27:F7:28:ARG:HA	27:F7:31:LYS:HG2	1.96	0.48
42:Fa:9:TRP:HZ2	60:CA:619:U:H5''	1.78	0.48
46:UA:21:UNK:HG1	57:UO:17:UNK:O	2.14	0.48
59:UY:98:UNK:HG2	59:UY:131:UNK:HB1	1.96	0.48
7:CQ:123:ARG:NH1	15:DD:727:PRO:O	2.47	0.47
23:F2:65:ARG:NH1	29:F9:40:ASP:OD1	2.46	0.47
24:F3:153:ILE:HG13	24:F3:238:LYS:HE2	1.96	0.47
37:FR:133:ASP:HB3	37:FR:240:LEU:HB3	1.96	0.47
59:UY:232:UNK:HA	59:UY:235:UNK:HG3	1.96	0.47
3:CH:196:ASP:H	23:F2:307:ASN:HD21	1.61	0.47
8:CR:121:TYR:O	8:CR:157:LYS:NZ	2.47	0.47
9:Ca:444:PHE:HB2	9:Ca:472:VAL:HG12	1.96	0.47
11:Cd:18:LEU:O	11:Cd:29:THR:OG1	2.30	0.47
23:F2:226:ARG:NH2	23:F2:266:GLU:OE2	2.47	0.47
28:F8:630:SER:OG	28:F8:633:GLU:OE1	2.30	0.47
37:FS:165:ARG:NH2	37:FS:179:CYS:O	2.45	0.47
38:FW:23:GLU:OE2	38:FW:27:ARG:NH2	2.47	0.47
1:CE:83:MET:HE3	1:CE:83:MET:HB3	1.83	0.47
9:Ca:548:GLU:HG2	36:FP:127:ARG:HH12	1.79	0.47
11:Cd:152:PRO:HG2	11:Cd:155:GLN:HB2	1.96	0.47
14:Cp:12:THR:HA	34:FM:63:ARG:HG3	1.96	0.47
28:F8:24:GLU:O	61:F1:1039:ARG:NH2	2.47	0.47
28:F8:219:HIS:HD2	28:F8:221:GLY:H	1.61	0.47
32:FE:153:ALA:O	37:FT:143:ARG:NE	2.48	0.47
35:FO:295:ARG:NH2	35:FO:309:ARG:O	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:Fa:72:GLU:O	42:Fa:75:ARG:NH1	2.47	0.47
7:CQ:87:GLN:NE2	7:CQ:93:ASP:O	2.48	0.47
24:F3:545:LEU:HD23	24:F3:594:GLU:HB3	1.96	0.47
24:F3:889:LEU:O	24:F3:893:LYS:NZ	2.47	0.47
25:F5:752:ASP:OD1	25:F5:752:ASP:N	2.48	0.47
28:F8:389:PRO:HB3	28:F8:641:THR:HA	1.94	0.47
28:F8:494:THR:HG23	28:F8:683:VAL:HG13	1.96	0.47
43:Fb:80:ILE:HG23	43:Fb:139:ILE:HG22	1.96	0.47
2:CF:151:ARG:NH2	26:F6:305:CYS:SG	2.87	0.47
9:Ca:67:ARG:NH1	9:Ca:181:GLU:OE2	2.47	0.47
16:DI:27:THR:H	16:DI:30:GLN:HE21	1.63	0.47
21:DU:165:ASP:OD1	21:DU:165:ASP:N	2.47	0.47
34:FN:216:GLU:O	34:FN:247:ARG:NH2	2.47	0.47
35:FO:113:ARG:HE	54:UI:5:UNK:HB1	1.78	0.47
37:FS:219:TYR:HE1	37:FS:248:ARG:HD2	1.78	0.47
5:CO:101:GLY:HA2	5:CO:105:ASN:HB2	1.97	0.47
8:CR:75:GLN:NE2	10:Cb:113:TYR:O	2.48	0.47
20:DR:41:HIS:ND1	20:DR:110:TYR:OH	2.43	0.47
23:F2:764:ASP:OD2	34:FM:63:ARG:NH2	2.43	0.47
30:FA:251:THR:HB	47:UB:7:UNK:HG1	1.97	0.47
35:FO:102:ILE:HG13	35:FO:288:VAL:HG13	1.96	0.47
37:FS:129:VAL:HG11	37:FS:210:LEU:HD21	1.96	0.47
59:UY:17:UNK:HG3	59:UY:76:UNK:HG2	1.95	0.47
59:UY:328:UNK:O	59:UY:332:UNK:HG3	2.14	0.47
2:CF:101:PRO:HD2	2:CF:104:ILE:HD12	1.97	0.47
6:CP:108:CYS:O	11:Cd:58:ARG:NH2	2.46	0.47
21:DU:113:GLN:HE21	24:F3:523:THR:HB	1.79	0.47
24:F3:654:GLN:HE21	24:F3:704:TYR:HE1	1.61	0.47
25:F5:723:ARG:HG3	25:F5:728:LEU:HB2	1.96	0.47
25:F5:739:ASN:OD1	25:F5:739:ASN:N	2.47	0.47
27:F7:146:THR:HB	27:F7:149:ARG:HG3	1.97	0.47
28:F8:175:VAL:HG21	28:F8:309:ALA:HB3	1.97	0.47
28:F8:544:ARG:NH2	32:FE:37:ASP:OD2	2.46	0.47
31:FB:444:ARG:NH1	37:FT:235:THR:OG1	2.45	0.47
59:UY:297:UNK:HB1	59:UY:315:UNK:HG3	1.97	0.47
3:CH:45:VAL:HG21	60:CA:315:A:H5"	1.97	0.47
5:CO:164:ARG:HH21	5:CO:215:ASP:HA	1.80	0.47
15:DD:607:GLN:O	20:DR:227:ARG:NH2	2.48	0.47
26:F6:344:LEU:HD21	26:F6:386:GLN:HA	1.96	0.47
28:F8:157:ALA:N	28:F8:391:CYS:O	2.48	0.47
32:FE:49:VAL:HG12	32:FE:97:LEU:HD22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CF:123:ARG:NH2	5:CO:141:GLY:O	2.48	0.47
5:CO:382:GLU:OE2	24:F3:457:SER:OG	2.29	0.47
14:Cp:37:GLN:NE2	38:FW:189:LEU:O	2.48	0.47
23:F2:475:ARG:NH2	23:F2:880:TYR:O	2.40	0.47
37:FT:73:THR:HG23	37:FT:75:GLN:H	1.79	0.47
59:UY:205:UNK:HA	59:UY:208:UNK:HG2	1.96	0.47
2:CF:144:MET:HE1	10:Cb:104:LEU:HD12	1.96	0.47
17:DL:139:ARG:O	17:DL:143:ASN:ND2	2.40	0.47
25:F5:707:VAL:HG11	44:Fc:85:LYS:HG3	1.96	0.47
34:FN:200:ASN:OD1	34:FN:238:ASN:ND2	2.48	0.47
37:FS:251:ARG:HH12	37:FU:252:VAL:HG21	1.80	0.47
5:CO:261:HIS:ND1	5:CO:303:TYR:OH	2.48	0.46
9:Ca:280:GLU:HA	9:Ca:379:MET:HE3	1.96	0.46
23:F2:857:ALA:O	29:F9:165:ARG:NH2	2.49	0.46
30:FA:102:LEU:HB2	55:UJ:4:UNK:HG1	1.96	0.46
36:FP:326:THR:HB	36:FP:329:HIS:HB3	1.96	0.46
37:FS:282:PRO:HG2	37:FS:284:ARG:HH21	1.81	0.46
59:UY:85:UNK:HG1	59:UY:134:UNK:HG2	1.96	0.46
10:Cb:167:GLU:HB3	26:F6:257:LEU:HD22	1.97	0.46
15:DD:390:VAL:HG13	15:DD:457:LEU:HD22	1.97	0.46
36:FP:262:ARG:NH1	36:FP:267:ASP:OD1	2.48	0.46
37:FS:227:THR:HB	37:FS:241:ILE:HB	1.96	0.46
37:FU:219:TYR:HB3	37:FU:246:PHE:HB3	1.97	0.46
40:FY:174:ASP:HB3	40:FY:177:ILE:HG13	1.96	0.46
1:CE:142:LEU:HD11	1:CE:167:LEU:HD22	1.97	0.46
8:CR:217:ARG:NH1	26:F6:421:ASP:OD1	2.49	0.46
10:Cb:191:HIS:CB	46:UA:13:UNK:HG3	2.45	0.46
15:DD:349:CYS:SG	15:DD:362:ASN:ND2	2.85	0.46
15:DD:421:PHE:HB3	15:DD:531:LYS:HG3	1.97	0.46
35:FO:25:TRP:CH2	49:UD:5:UNK:O	2.67	0.46
35:FO:70:MET:HG3	35:FO:75:VAL:HG13	1.97	0.46
59:UY:198:UNK:HG1	59:UY:226:UNK:HG1	1.98	0.46
19:DP:91:GLU:OE2	19:DP:124:ARG:NH1	2.48	0.46
23:F2:666:ASP:OD1	23:F2:670:ASN:N	2.49	0.46
23:F2:741:ASP:OD1	23:F2:741:ASP:N	2.48	0.46
27:F7:327:GLU:O	27:F7:330:LYS:HB3	2.16	0.46
28:F8:644:ASP:OD1	28:F8:644:ASP:N	2.48	0.46
30:FA:608:ILE:HG12	30:FA:623:LEU:HB3	1.97	0.46
37:FR:139:GLN:HG3	60:CA:563:U:H1'	1.97	0.46
40:FY:165:GLN:HE22	60:CA:297:G:H2'	1.80	0.46
9:Ca:335:ARG:HE	15:DD:779:MET:HE2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Ca:485:MET:HE3	9:Ca:489:ARG:HD2	1.97	0.46
16:DI:191:VAL:HG23	16:DI:192:THR:HG23	1.96	0.46
17:DL:199:ASP:OD1	17:DL:214:TYR:OH	2.31	0.46
31:FC:353:ASP:HB3	31:FC:356:LEU:HB2	1.98	0.46
37:FS:35:PRO:HA	37:FS:38:GLN:HG2	1.97	0.46
37:FS:84:GLN:OE1	37:FU:75:GLN:NE2	2.47	0.46
60:CA:308:C:H2'	60:CA:309:A:H8	1.81	0.46
2:CF:119:ASP:OD1	11:CD:141:ARG:NE	2.48	0.46
12:Cj:23:GLY:O	20:DR:250:ARG:NH2	2.47	0.46
23:F2:615:ARG:HH11	60:CA:16:U:H2'	1.81	0.46
27:F7:147:PRO:HA	27:F7:150:LEU:HB2	1.97	0.46
31:FB:280:VAL:HG12	31:FB:557:LEU:HB3	1.97	0.46
35:FO:132:THR:OG1	37:FQ:178:GLN:NE2	2.48	0.46
36:FP:85:LYS:HA	36:FP:85:LYS:HD2	1.54	0.46
25:F5:187:HIS:O	29:F9:204:LYS:NZ	2.49	0.46
59:UY:341:UNK:HG2	59:UY:409:UNK:HG2	1.98	0.46
2:CF:51:PHE:HB2	2:CF:90:LEU:HD13	1.97	0.46
15:DD:801:GLU:OE2	21:DU:221:TYR:OH	2.33	0.46
27:F7:352:GLU:OE1	27:F7:382:SER:OG	2.31	0.46
28:F8:47:PHE:HB3	28:F8:557:LEU:HD22	1.98	0.46
37:FU:155:PHE:HD1	37:FU:217:MET:HE3	1.81	0.46
4:CK:281:VAL:H	4:CK:309:ASP:HA	1.80	0.46
11:CD:24:HIS:NE2	60:CA:51:U:O2'	2.39	0.46
17:DL:132:ASN:O	17:DL:138:SER:OG	2.28	0.46
24:F3:297:PHE:HB2	24:F3:314:THR:HG23	1.96	0.46
7:CQ:118:PRO:O	60:CA:146:U:O2'	2.34	0.46
16:DI:218:ASP:OD1	16:DI:218:ASP:N	2.48	0.46
25:F5:640:GLU:O	43:Fb:115:LYS:NZ	2.49	0.46
34:FN:15:MET:HE3	34:FN:38:ILE:HG23	1.98	0.46
7:CQ:86:ASN:O	15:DD:128:ASN:ND2	2.47	0.45
9:Ca:92:ILE:HD11	50:UP:4:UNK:HB1	1.98	0.45
24:F3:896:ALA:HB2	24:F3:957:MET:HB3	1.97	0.45
26:F6:132:ASP:OD2	26:F6:136:ARG:NH1	2.49	0.45
34:FM:13:VAL:HB	34:FM:80:LEU:HG	1.99	0.45
59:UY:99:UNK:HG2	59:UY:255:UNK:HG2	1.98	0.45
59:UY:119:UNK:HA	59:UY:133:UNK:HA	1.97	0.45
11:CD:140:GLU:O	11:CD:144:ASN:ND2	2.49	0.45
15:DD:206:TRP:HE3	16:DI:61:ASN:HB3	1.81	0.45
20:DR:63:ILE:HG23	20:DR:64:ILE:HG13	1.99	0.45
21:DU:180:VAL:HG13	24:F3:530:HIS:HB3	1.98	0.45
27:F7:115:ARG:NH1	60:CA:326:U:O2'	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:F9:77:ALA:HB1	29:F9:182:GLU:HB2	1.98	0.45
32:FE:179:LEU:HB2	32:FE:183:LEU:HD23	1.98	0.45
32:FE:353:THR:O	32:FE:353:THR:OG1	2.29	0.45
37:FR:131:VAL:HB	37:FR:242:HIS:HB3	1.98	0.45
5:CO:174:PRO:HD2	5:CO:177:MET:HE3	1.99	0.45
9:Ca:91:ASP:OD1	9:Ca:91:ASP:N	2.39	0.45
19:DP:46:LEU:HD11	35:FO:188:SER:HB2	1.97	0.45
22:DZ:67:GLU:HG3	22:DZ:69:HIS:H	1.81	0.45
24:F3:164:TYR:HB3	49:UD:6:UNK:HG2	1.99	0.45
25:F5:701:LEU:HD21	44:Fc:82:ASN:HB2	1.98	0.45
31:FB:268:VAL:HG23	31:FB:287:VAL:HG22	1.97	0.45
32:FE:240:LYS:NZ	32:FE:245:PRO:O	2.49	0.45
33:FJ:68:LEU:O	33:FJ:77:ARG:NH1	2.44	0.45
59:UY:74:UNK:O	59:UY:132:UNK:HG1	2.16	0.45
60:CA:195:A:H3'	60:CA:196:U:H2'	1.98	0.45
12:Cj:81:GLU:HA	12:Cj:84:ARG:HG2	1.97	0.45
14:Cp:26:ASP:OD2	14:Cp:28:ARG:NE	2.48	0.45
20:DR:47:HIS:HB3	20:DR:192:LEU:HD12	1.98	0.45
25:F5:655:SER:OG	25:F5:658:ASP:OD2	2.34	0.45
33:FJ:10:VAL:HB	33:FJ:14:THR:HB	1.98	0.45
15:DD:94:LYS:HG3	60:CA:144:A:H5''	1.98	0.45
17:DL:306:PRO:HB2	33:FJ:98:ARG:HG2	1.97	0.45
34:FM:320:GLU:HG2	49:UQ:4:UNK:HG1	1.98	0.45
38:FW:15:ASN:OD1	38:FW:19:THR:OG1	2.34	0.45
39:FX:48:HIS:NE2	48:UC:10:UNK:HG3	2.32	0.45
28:F8:92:VAL:HB	28:F8:113:ARG:HB2	1.98	0.45
31:FB:335:LEU:HD13	31:FB:563:PRO:HD3	1.98	0.45
33:FJ:298:LYS:HA	33:FJ:298:LYS:HD3	1.76	0.45
43:Fb:128:HIS:HB2	50:UP:36:UNK:HB2	1.98	0.45
60:CA:130:U:H2'	60:CA:131:A:H8	1.82	0.45
24:F3:857:MET:HE2	24:F3:857:MET:HB3	1.89	0.45
25:F5:612:GLU:HA	25:F5:615:THR:HG22	1.97	0.45
34:FN:31:ARG:HD3	34:FN:59:THR:HG21	1.99	0.45
2:CF:15:ARG:NH2	11:Cd:165:ASP:OD1	2.49	0.45
9:Ca:254:ARG:NH2	22:DZ:91:ASP:OD1	2.50	0.45
14:Cp:46:ILE:HA	14:Cp:113:GLN:HE22	1.80	0.45
15:DD:425:LYS:HA	15:DD:425:LYS:HD3	1.83	0.45
30:FA:244:GLU:OE1	30:FA:247:ARG:NH2	2.50	0.45
31:FC:505:HIS:HD2	31:FC:549:THR:HG21	1.81	0.45
32:FE:134:TRP:HA	32:FE:138:LEU:HB2	1.99	0.45
32:FE:145:TYR:OH	32:FE:192:PRO:O	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:FP:73:PRO:HA	38:FW:217:ARG:HH21	1.81	0.45
9:Ca:62:TRP:O	9:Ca:94:TRP:NE1	2.48	0.45
24:F3:412:TYR:HA	24:F3:416:GLU:HB3	1.97	0.45
26:F6:192:VAL:HG23	26:F6:193:GLN:HG3	1.99	0.45
27:F7:431:LEU:HD23	27:F7:431:LEU:HA	1.87	0.45
32:FE:365:HIS:HB3	32:FE:368:GLU:HB2	1.99	0.45
35:FO:6:ARG:NH1	35:FO:39:GLY:O	2.50	0.45
59:UY:56:UNK:HA	59:UY:57:UNK:HA	1.99	0.45
59:UY:235:UNK:HA	59:UY:238:UNK:HG3	1.99	0.45
16:DI:74:ASP:OD1	16:DI:74:ASP:N	2.49	0.45
17:DL:183:LEU:HD11	17:DL:230:PRO:HB2	1.99	0.45
23:F2:953:GLU:HG3	29:F9:126:ARG:HH12	1.81	0.45
29:F9:146:MET:HE1	29:F9:177:PRO:HG3	1.99	0.45
7:CQ:176:LYS:O	27:F7:380:ARG:NH2	2.50	0.44
7:CQ:210:LEU:HA	27:F7:70:LEU:HD13	1.99	0.44
8:CR:173:ARG:HD2	40:FY:137:THR:HG21	1.98	0.44
26:F6:58:PHE:HE2	26:F6:60:LEU:HD13	1.82	0.44
27:F7:187:ALA:HB1	60:CA:292:U:H1'	2.00	0.44
27:F7:287:ARG:HB2	27:F7:290:MET:HG3	1.99	0.44
36:FP:15:ASN:HD22	36:FP:17:TYR:H	1.65	0.44
46:UA:10:UNK:O	46:UA:13:UNK:HB2	2.16	0.44
54:UN:4:UNK:HB2	54:UN:5:UNK:HG3	1.98	0.44
59:UY:242:UNK:HB2	59:UY:248:UNK:HG1	1.99	0.44
11:Cd:128:GLU:OE1	18:DO:190:TYR:OH	2.32	0.44
12:Cj:61:ASP:OD1	12:Cj:61:ASP:N	2.46	0.44
25:F5:406:ILE:HA	25:F5:409:ARG:HD2	1.99	0.44
26:F6:403:LEU:HD22	26:F6:415:VAL:HG11	1.99	0.44
28:F8:432:MET:O	28:F8:433:ARG:NH1	2.47	0.44
30:FA:142:MET:HB3	62:FF:1:MET:H1	1.82	0.44
30:FA:526:THR:HB	30:FA:538:PRO:HA	1.98	0.44
32:FE:42:VAL:HG11	32:FE:70:GLY:HA3	1.98	0.44
2:CF:105:ARG:NH2	60:CA:309:A:OP2	2.51	0.44
6:CP:172:VAL:O	9:Ca:541:ARG:NH2	2.41	0.44
16:DI:138:GLU:HG2	39:FX:67:ARG:HD2	1.99	0.44
23:F2:64:GLU:HB2	29:F9:47:ARG:HH21	1.80	0.44
33:FJ:249:VAL:O	33:FJ:252:ARG:NH1	2.47	0.44
34:FM:72:THR:O	34:FM:107:GLN:NE2	2.45	0.44
37:FS:36:PHE:HB2	37:FS:96:TRP:HB3	1.99	0.44
37:FT:133:ASP:HB3	37:FT:240:LEU:HB3	1.98	0.44
16:DI:250:ASN:O	16:DI:262:LYS:NZ	2.51	0.44
28:F8:89:GLY:HA2	28:F8:115:TYR:HE1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:FA:116:VAL:HB	30:FA:120:MET:HG3	1.98	0.44
37:FU:239:MET:HE2	37:FU:239:MET:HB3	1.86	0.44
59:UY:414:UNK:HG2	59:UY:416:UNK:HG3	1.99	0.44
9:Ca:60:ASP:OD1	9:Ca:60:ASP:N	2.50	0.44
27:F7:144:LEU:HD22	27:F7:150:LEU:HD11	2.00	0.44
27:F7:542:ASN:ND2	27:F7:580:CYS:SG	2.90	0.44
31:FC:189:VAL:HG12	31:FC:320:TYR:HD1	1.83	0.44
37:FQ:40:PHE:HA	37:FQ:41:PRO:HD3	1.87	0.44
5:CO:424:LYS:NZ	60:CA:130:U:OP2	2.46	0.44
10:Cb:116:PHE:O	10:Cb:157:LYS:NZ	2.41	0.44
12:Cj:13:PRO:O	20:DR:263:SER:OG	2.36	0.44
15:DD:665:GLU:OE1	15:DD:668:ARG:NH1	2.50	0.44
19:DP:24:LYS:HG2	60:CA:52:C:H3'	1.99	0.44
20:DR:240:PRO:HG3	20:DR:269:TRP:HB3	2.00	0.44
30:FA:434:GLN:HE22	30:FA:437:LEU:HB3	1.82	0.44
31:FB:336:ARG:HG2	31:FB:561:GLU:HB2	1.99	0.44
31:FC:293:ILE:HD12	31:FC:295:LEU:HB2	2.00	0.44
34:FN:36:LEU:HD23	34:FN:62:MET:HE2	1.98	0.44
38:FW:18:ARG:N	64:FWA:1:PO4:O3	2.50	0.44
1:CE:49:PRO:O	23:F2:786:ARG:NH2	2.46	0.44
1:CE:370:ASP:OD1	1:CE:370:ASP:N	2.50	0.44
5:CO:266:LEU:HG	5:CO:274:TYR:HB2	1.99	0.44
7:CQ:123:ARG:NH2	60:CA:321:A:OP2	2.51	0.44
14:Cp:182:GLN:NE2	19:DP:161:VAL:O	2.51	0.44
20:DR:129:ASP:N	20:DR:129:ASP:OD1	2.50	0.44
31:FC:337:ARG:NH1	31:FC:500:ARG:O	2.50	0.44
33:FJ:130:SER:H	33:FJ:133:ALA:HB3	1.83	0.44
35:FO:274:VAL:HA	35:FO:275:PRO:HD3	1.88	0.44
37:FU:138:ASP:N	37:FU:138:ASP:OD1	2.50	0.44
59:UY:218:UNK:HB1	59:UY:268:UNK:HG2	1.99	0.44
1:CE:302:PRO:O	1:CE:305:GLU:HB2	2.17	0.44
2:CF:14:GLN:OE1	2:CF:16:ARG:NH2	2.44	0.44
12:Cj:10:ARG:HH12	60:CA:76:A:H5''	1.82	0.44
16:DI:299:THR:HG21	16:DI:363:VAL:HG22	1.99	0.44
17:DL:292:ARG:O	60:CA:534:A:O2'	2.30	0.44
24:F3:693:LEU:HD23	24:F3:729:LEU:HD23	1.99	0.44
26:F6:64:ARG:HB3	26:F6:100:THR:HB	2.00	0.44
37:FS:58:ASP:HB2	37:FU:24:LEU:HD13	2.00	0.44
37:FS:143:ARG:HD2	37:FS:193:LYS:HE2	1.99	0.44
17:DL:240:GLU:OE2	17:DL:248:ARG:NH1	2.50	0.44
19:DP:54:LEU:HD13	19:DP:58:TYR:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:FA:372:ARG:HH21	30:FA:377:ALA:HA	1.83	0.44
34:FN:226:ASP:OD2	38:FW:80:TYR:OH	2.36	0.44
39:FX:93:ASP:OD1	39:FX:93:ASP:N	2.48	0.44
42:Fa:53:LYS:NZ	60:CA:619:U:OP1	2.42	0.44
45:Fd:97:LYS:HA	45:Fd:101:ARG:HB2	2.00	0.44
6:CP:81:PRO:HG2	36:FP:19:LYS:HG3	1.99	0.43
6:CP:131:ASN:OD1	60:CA:179:U:N3	2.40	0.43
8:CR:137:THR:OG1	8:CR:138:ARG:N	2.51	0.43
17:DL:207:THR:HG21	17:DL:213:SER:HB3	1.98	0.43
18:DO:139:GLU:OE2	18:DO:179:ARG:NH1	2.50	0.43
21:DU:111:ILE:HB	21:DU:143:PRO:HA	2.00	0.43
32:FE:72:ARG:NH2	60:CA:196:U:OP2	2.44	0.43
59:UY:235:UNK:HG2	59:UY:241:UNK:HB1	2.00	0.43
26:F6:5:ALA:HB1	26:F6:140:ILE:HG22	1.99	0.43
27:F7:351:ILE:HG13	27:F7:379:ILE:HG21	2.00	0.43
28:F8:222:LEU:O	28:F8:238:ARG:NH1	2.52	0.43
31:FB:181:PRO:HG2	31:FB:184:LEU:HD12	2.00	0.43
31:FC:333:SER:O	31:FC:500:ARG:NE	2.51	0.43
34:FN:40:SER:OG	34:FN:42:ALA:O	2.36	0.43
9:Ca:266:GLU:HB3	23:F2:731:PHE:HZ	1.83	0.43
20:DR:247:LEU:HD12	20:DR:249:GLU:HG2	2.00	0.43
30:FA:151:THR:OG1	30:FA:154:MET:SD	2.73	0.43
31:FC:575:ASP:OD1	31:FC:575:ASP:N	2.49	0.43
34:FM:24:ARG:HA	34:FM:53:LEU:HD21	2.00	0.43
35:FO:26:GLN:HB3	49:UD:4:UNK:HG1	2.01	0.43
38:FW:255:ARG:HG2	38:FW:258:LEU:HD12	2.00	0.43
59:UY:100:UNK:HA	59:UY:254:UNK:HB1	2.00	0.43
7:CQ:123:ARG:HH12	15:DD:727:PRO:HG2	1.83	0.43
12:Cj:72:ASP:OD1	12:Cj:75:SER:OG	2.34	0.43
14:Cp:20:LYS:NZ	34:FM:32:SER:OG	2.49	0.43
23:F2:88:ASN:HD22	23:F2:200:VAL:HG12	1.83	0.43
23:F2:894:PHE:O	23:F2:939:LYS:NZ	2.43	0.43
31:FB:301:ILE:HG23	31:FB:317:ILE:HB	2.00	0.43
34:FM:68:TYR:O	34:FM:72:THR:OG1	2.34	0.43
50:UE:15:UNK:HA	50:UE:18:UNK:HG3	2.00	0.43
15:DD:621:LEU:O	15:DD:624:THR:OG1	2.29	0.43
20:DR:158:ARG:HH21	20:DR:172:SER:HA	1.83	0.43
24:F3:952:LEU:HB3	24:F3:958:SER:HB3	2.01	0.43
25:F5:749:ILE:HD12	43:Fb:133:LYS:HD3	2.01	0.43
34:FM:204:ALA:HB1	34:FM:311:VAL:HG12	2.00	0.43
37:FT:82:ASN:OD1	37:FT:82:ASN:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:FU:23:THR:OG1	37:FU:24:LEU:N	2.50	0.43
59:UY:117:UNK:HG2	60:CA:351:A:H4'	2.01	0.43
59:UY:188:UNK:HB2	59:UY:193:UNK:CB	2.46	0.43
59:UY:192:UNK:C	59:UY:278:UNK:HB1	2.49	0.43
61:F1:994:ASP:OD1	61:F1:998:ARG:NH2	2.51	0.43
2:CF:119:ASP:OD2	11:Cd:137:ARG:NH2	2.46	0.43
20:DR:237:TYR:OH	20:DR:269:TRP:O	2.31	0.43
25:F5:206:LYS:HA	25:F5:206:LYS:HD3	1.84	0.43
25:F5:352:LYS:HD3	25:F5:352:LYS:HA	1.77	0.43
26:F6:213:PHE:HA	26:F6:248:VAL:H	1.83	0.43
26:F6:423:THR:HG23	26:F6:426:GLU:H	1.84	0.43
28:F8:123:TYR:HE2	28:F8:163:ALA:HB2	1.84	0.43
30:FA:295:SER:OG	30:FA:296:GLN:OE1	2.33	0.43
30:FA:405:ALA:HA	30:FA:408:ILE:HD12	1.99	0.43
31:FB:313:GLN:HA	31:FB:314:PRO:HD3	1.87	0.43
31:FB:336:ARG:HA	31:FB:500:ARG:HA	2.01	0.43
37:FS:146:LEU:HD13	37:FS:189:PHE:HD2	1.83	0.43
43:Fb:134:GLN:HE21	43:Fb:134:GLN:HB3	1.55	0.43
60:CA:341:A:H2	60:CA:342:A:H62	1.65	0.43
9:Ca:251:LYS:HB2	23:F2:809:SER:HB3	2.01	0.43
11:Cd:26:ARG:NH2	60:CA:48:U:OP2	2.50	0.43
12:Cj:156:THR:HG21	12:Cj:190:PRO:HG2	2.01	0.43
20:DR:252:ALA:HA	20:DR:262:ARG:HG3	2.00	0.43
25:F5:378:PRO:HG2	25:F5:478:GLN:HG3	1.99	0.43
28:F8:101:THR:OG1	28:F8:102:GLY:N	2.52	0.43
30:FA:586:SER:OG	31:FB:322:ARG:NH2	2.52	0.43
31:FB:199:ASP:HB3	31:FB:248:HIS:HD2	1.84	0.43
31:FC:375:ALA:O	31:FC:380:LYS:NZ	2.38	0.43
31:FC:392:ASN:HD21	31:FC:539:ARG:HD3	1.83	0.43
34:FN:276:LYS:HE3	34:FN:276:LYS:HB3	1.83	0.43
37:FQ:211:VAL:HG12	37:FQ:246:PHE:HZ	1.84	0.43
59:UY:171:UNK:HG2	59:UY:173:UNK:HG3	2.01	0.43
59:UY:185:UNK:HA	59:UY:196:UNK:HA	2.01	0.43
59:UY:277:UNK:HB1	59:UY:289:UNK:HB2	2.01	0.43
59:UY:440:UNK:HG2	59:UY:441:UNK:HG2	2.00	0.43
4:CK:316:ASN:HB2	40:FY:166:HIS:CE1	2.54	0.43
5:CO:178:LEU:H	5:CO:178:LEU:HG	1.67	0.43
5:CO:318:VAL:HG12	5:CO:319:MET:HG3	2.01	0.43
9:Ca:75:LEU:HD12	9:Ca:180:ASN:HB2	2.00	0.43
16:DI:82:GLU:OE2	16:DI:221:TYR:OH	2.34	0.43
27:F7:237:ARG:NH2	45:Fd:96:GLU:OE1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:FR:224:SER:HB3	37:FR:242:HIS:HE1	1.84	0.43
37:FR:237:VAL:O	37:FS:238:ARG:NH2	2.52	0.43
37:FT:125:ASP:OD1	37:FT:125:ASP:N	2.49	0.43
60:CA:361:A:H2'	60:CA:362:A:C8	2.54	0.43
4:CK:288:ARG:HH21	33:FJ:199:THR:HA	1.84	0.43
16:DI:262:LYS:HE2	16:DI:262:LYS:HB2	1.83	0.43
30:FA:187:PRO:HG3	47:UB:2:UNK:CG	2.49	0.43
32:FE:114:ASN:HD21	37:FQ:139:GLN:HE21	1.67	0.43
37:FT:143:ARG:NH1	37:FT:144:HIS:O	2.51	0.43
50:UE:7:UNK:HA	50:UE:10:UNK:HG3	2.00	0.43
59:UY:89:UNK:HG1	59:UY:136:UNK:HG2	2.01	0.43
1:CE:107:LYS:HE3	29:F9:142:PRO:HD2	2.01	0.43
5:CO:251:VAL:O	5:CO:255:THR:OG1	2.32	0.43
9:Ca:205:LEU:HD22	23:F2:811:LEU:HD22	2.00	0.43
9:Ca:243:THR:OG1	9:Ca:245:GLU:OE1	2.36	0.43
24:F3:226:LEU:HD21	24:F3:285:ALA:HB1	2.00	0.43
27:F7:482:LEU:HD23	27:F7:482:LEU:HA	1.90	0.43
31:FB:495:ILE:HD12	31:FB:511:VAL:HG22	2.00	0.43
59:UY:445:UNK:HA	59:UY:448:UNK:HG3	2.01	0.43
6:CP:66:LYS:H	6:CP:93:THR:HG23	1.83	0.42
16:DI:47:LEU:HD21	16:DI:200:ARG:HH22	1.84	0.42
27:F7:127:ARG:HA	27:F7:127:ARG:HD2	1.92	0.42
27:F7:190:GLN:HA	27:F7:193:VAL:HG12	2.01	0.42
30:FA:112:HIS:HB3	30:FA:115:ALA:HB3	2.01	0.42
32:FE:187:TYR:HB3	32:FE:267:MET:HE3	2.01	0.42
32:FE:269:ARG:HH21	60:CA:254:A:H5'	1.84	0.42
33:FJ:197:ASP:OD2	33:FJ:199:THR:OG1	2.37	0.42
6:CP:11:ALA:O	19:DP:15:ARG:NE	2.51	0.42
17:DL:161:THR:HA	17:DL:164:ARG:HD2	2.01	0.42
25:F5:188:ARG:HE	41:FZ:19:ASN:HB3	1.84	0.42
25:F5:723:ARG:O	25:F5:727:GLY:N	2.43	0.42
30:FA:43:PHE:HD2	30:FA:72:ILE:HD12	1.85	0.42
35:FO:216:LEU:HG	49:UM:6:UNK:HG3	2.02	0.42
37:FQ:238:ARG:NH2	37:FT:230:PRO:O	2.52	0.42
43:Fb:128:HIS:CG	50:UP:36:UNK:HB2	2.54	0.42
21:DU:174:ARG:HH21	21:DU:178:TRP:HD1	1.66	0.42
26:F6:215:ARG:HB3	57:UO:20:UNK:HB1	1.99	0.42
26:F6:263:ILE:HD12	26:F6:264:PRO:HD2	2.01	0.42
59:UY:93:UNK:O	59:UY:135:UNK:N	2.52	0.42
59:UY:219:UNK:O	59:UY:222:UNK:HG3	2.20	0.42
59:UY:296:UNK:O	59:UY:299:UNK:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Cp:23:TYR:OH	34:FM:51:ASP:OD1	2.32	0.42
15:DD:300:GLN:O	15:DD:303:LEU:HB3	2.19	0.42
23:F2:949:LEU:HD21	25:F5:446:LEU:HD22	2.00	0.42
33:FJ:165:SER:O	33:FJ:273:ARG:NH2	2.52	0.42
34:FM:292:ARG:HH12	34:FM:321:LEU:HD22	1.85	0.42
35:FO:19:MET:HE3	35:FO:19:MET:HB2	1.92	0.42
37:FT:93:MET:O	37:FT:98:LEU:N	2.52	0.42
38:FW:50:LEU:HD22	38:FW:222:GLU:HG3	2.01	0.42
42:Fa:140:ALA:O	42:Fa:146:ARG:NH1	2.52	0.42
45:Fd:59:HIS:CD2	45:Fd:62:LEU:H	2.37	0.42
59:UY:86:UNK:O	59:UY:89:UNK:HG3	2.18	0.42
59:UY:151:UNK:HA	59:UY:154:UNK:HG3	2.01	0.42
1:CE:143:ASN:ND2	1:CE:168:TYR:OH	2.48	0.42
2:CF:35:LEU:HD11	5:CO:187:LYS:HB3	2.01	0.42
12:Cj:102:GLN:HA	19:DP:143:ASN:HD21	1.84	0.42
22:DZ:70:HIS:N	23:F2:773:ASP:OD2	2.51	0.42
26:F6:225:ALA:HA	26:F6:229:LEU:HD12	2.00	0.42
28:F8:696:GLN:NE2	28:F8:719:ASN:O	2.52	0.42
30:FA:152:LEU:HD23	30:FA:155:LEU:HD12	2.00	0.42
32:FE:287:ASP:OD1	32:FE:287:ASP:N	2.42	0.42
32:FE:405:PRO:HD2	32:FE:408:MET:HE3	2.01	0.42
46:UA:6:UNK:HA	46:UA:9:UNK:HG3	2.02	0.42
2:CF:50:ARG:HB2	40:FY:136:GLU:HB2	2.02	0.42
5:CO:183:ASP:OD1	5:CO:183:ASP:N	2.52	0.42
7:CQ:102:SER:HB3	60:CA:121:A:H5'	2.00	0.42
20:DR:255:PRO:HG2	20:DR:260:GLY:HA3	2.00	0.42
27:F7:127:ARG:NE	59:UY:297:UNK:O	2.52	0.42
35:FO:96:TRP:CE2	35:FO:101:ARG:HD3	2.55	0.42
35:FO:250:LEU:HB2	35:FO:255:GLN:HB2	2.02	0.42
59:UY:114:UNK:HG2	59:UY:121:UNK:HG2	2.00	0.42
60:CA:315:A:H2'	60:CA:316:A:C8	2.55	0.42
3:CH:41:VAL:HG21	3:CH:47:ARG:HG2	2.01	0.42
5:CO:233:ARG:NE	27:F7:181:GLU:OE1	2.47	0.42
16:DI:27:THR:HG22	16:DI:30:GLN:HE21	1.83	0.42
24:F3:806:TYR:O	24:F3:810:THR:OG1	2.38	0.42
28:F8:509:PRO:HD3	28:F8:608:TRP:HA	2.02	0.42
30:FA:272:VAL:HG23	30:FA:353:LYS:HD3	2.01	0.42
30:FA:361:ALA:HB2	30:FA:404:LEU:HD21	2.01	0.42
45:Fd:59:HIS:HD2	45:Fd:61:GLU:H	1.67	0.42
59:UY:284:UNK:HG3	59:UY:432:UNK:HG3	2.02	0.42
60:CA:590:A:H2'	60:CA:591:A:C8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:CR:149:PRO:HB2	42:Fa:13:VAL:HB	2.01	0.42
15:DD:243:GLU:HB2	15:DD:246:GLU:HG3	2.01	0.42
16:DI:121:LYS:HD3	16:DI:121:LYS:HA	1.80	0.42
17:DL:125:HIS:HA	17:DL:128:MET:HE3	2.02	0.42
23:F2:105:SER:O	23:F2:120:TYR:OH	2.36	0.42
23:F2:417:ARG:NH1	23:F2:878:SER:O	2.48	0.42
35:FO:61:LEU:HD12	35:FO:109:ILE:HD11	2.02	0.42
37:FQ:225:TYR:CZ	37:FR:226:VAL:HB	2.55	0.42
37:FT:10:ASP:OD1	37:FT:10:ASP:N	2.48	0.42
39:FX:112:GLU:HA	39:FX:115:LYS:HG2	2.02	0.42
59:UY:55:UNK:HG2	59:UY:58:UNK:HG3	2.01	0.42
59:UY:150:UNK:HG2	59:UY:295:UNK:HB2	2.02	0.42
9:Ca:61:LEU:HD12	25:F5:693:TRP:HA	2.02	0.42
12:Cj:119:LYS:HB2	12:Cj:172:TYR:HE2	1.84	0.42
24:F3:188:ARG:O	24:F3:257:ARG:NH2	2.53	0.42
42:Fa:98:LEU:HD13	42:Fa:107:VAL:HG21	2.01	0.42
8:CR:80:LEU:HD13	8:CR:80:LEU:HA	1.95	0.42
10:Cb:120:LYS:HA	26:F6:197:THR:HG21	2.02	0.42
12:Cj:126:TYR:HD2	20:DR:268:HIS:HA	1.85	0.42
15:DD:414:ARG:NH1	15:DD:514:ASP:OD1	2.47	0.42
32:FE:183:LEU:HA	32:FE:184:PRO:HD3	1.92	0.42
33:FJ:163:GLU:O	33:FJ:171:ARG:NE	2.53	0.42
42:Fa:28:MET:HB2	42:Fa:52:MET:HE2	2.02	0.42
45:Fd:93:MET:HE3	45:Fd:93:MET:HB3	1.95	0.42
1:CE:103:GLY:O	1:CE:105:GLN:NE2	2.52	0.41
5:CO:318:VAL:O	27:F7:411:ARG:NH2	2.49	0.41
21:DU:177:ASP:OD1	21:DU:177:ASP:N	2.45	0.41
23:F2:532:ASP:OD2	60:CA:10:G:N1	2.53	0.41
23:F2:768:LEU:H	23:F2:768:LEU:HG	1.62	0.41
26:F6:437:ILE:HG21	26:F6:474:GLY:HA3	2.00	0.41
28:F8:122:ALA:HB3	32:FE:407:GLU:HG3	2.02	0.41
28:F8:505:SER:O	28:F8:610:TYR:HA	2.20	0.41
30:FA:134:TRP:HB3	30:FA:162:CYS:HA	2.02	0.41
30:FA:338:SER:O	30:FA:342:THR:OG1	2.36	0.41
30:FA:561:ASN:HD21	30:FA:629:ALA:HB1	1.84	0.41
31:FC:361:ASP:OD1	31:FC:361:ASP:N	2.46	0.41
31:FC:384:TYR:HA	31:FC:546:ARG:HH21	1.85	0.41
31:FC:505:HIS:O	31:FC:509:ASN:ND2	2.53	0.41
36:FP:86:SER:OG	36:FP:87:GLY:N	2.53	0.41
37:FR:35:PRO:HD2	37:FR:97:GLY:HA3	2.02	0.41
59:UY:54:UNK:HG3	59:UY:398:UNK:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:DD:126:MET:HE3	15:DD:126:MET:HB2	1.92	0.41
29:F9:171:LEU:HD13	29:F9:176:LEU:HD11	2.02	0.41
31:FC:340:VAL:HG12	31:FC:558:TRP:HB2	2.01	0.41
32:FE:306:GLN:HB3	32:FE:311:LEU:HD11	2.01	0.41
34:FM:62:MET:HE2	34:FM:62:MET:HB3	1.87	0.41
37:FS:135:MET:HE2	37:FS:135:MET:HB3	1.75	0.41
59:UY:198:UNK:HG2	59:UY:272:UNK:HG2	2.01	0.41
59:UY:227:UNK:HB2	59:UY:290:UNK:HG1	2.03	0.41
4:CK:187:ARG:HE	26:F6:478:VAL:HG21	1.84	0.41
9:Ca:113:LEU:HD22	9:Ca:120:ASN:HA	2.02	0.41
9:Ca:252:ARG:HD2	9:Ca:252:ARG:HA	1.91	0.41
17:DL:171:ARG:HH22	17:DL:242:ARG:HE	1.66	0.41
24:F3:392:CYS:HB3	24:F3:504:ARG:HE	1.86	0.41
26:F6:244:MET:HE2	26:F6:287:ARG:HB2	2.01	0.41
30:FA:147:ASN:HD21	62:FF:4:ILE:H	1.68	0.41
60:CA:27:A:O2'	60:CA:28:U:O4'	2.36	0.41
4:CK:200:ARG:HH21	40:FY:177:ILE:HG22	1.86	0.41
5:CO:421:TRP:CD1	60:CA:105:G:H5'	2.56	0.41
10:Cb:107:SER:OG	10:Cb:108:GLU:OE1	2.37	0.41
15:DD:561:ASP:OD1	15:DD:561:ASP:N	2.52	0.41
26:F6:45:PHE:O	26:F6:119:ARG:NH2	2.48	0.41
27:F7:386:PHE:HA	27:F7:389:LEU:HB2	2.02	0.41
27:F7:472:THR:H	27:F7:475:MET:HE3	1.86	0.41
30:FA:583:LEU:HB2	30:FA:586:SER:HB3	2.02	0.41
31:FB:194:GLN:HA	31:FC:352:PHE:HE1	1.86	0.41
35:FO:160:LEU:HD11	35:FO:193:LEU:HD21	2.02	0.41
37:FU:217:MET:HE2	37:FU:217:MET:HB2	1.96	0.41
38:FW:155:ARG:HG3	38:FW:190:ARG:HH21	1.85	0.41
1:CE:326:MET:HB2	1:CE:329:ARG:HG2	2.03	0.41
7:CQ:122:GLN:HE21	27:F7:660:VAL:HG13	1.85	0.41
10:Cb:191:HIS:HB3	46:UA:13:UNK:HG3	2.02	0.41
16:DI:41:LYS:HD2	16:DI:41:LYS:HA	1.83	0.41
19:DP:90:LEU:HD13	19:DP:127:ASP:HB3	2.03	0.41
24:F3:650:GLN:HG3	27:F7:401:ASP:HB3	2.02	0.41
26:F6:142:SER:HA	26:F6:145:GLU:HG2	2.01	0.41
27:F7:566:LYS:HA	27:F7:566:LYS:HD3	1.78	0.41
31:FC:196:ASN:O	31:FC:246:ARG:NH1	2.45	0.41
31:FC:512:SER:HA	31:FC:515:LYS:HG2	2.03	0.41
32:FE:199:SER:OG	32:FE:392:THR:O	2.31	0.41
37:FU:258:ASP:OD1	37:FU:258:ASP:N	2.53	0.41
43:Fb:140:MET:HE3	43:Fb:143:ARG:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:CA:236:G:N2	60:CA:241:U:H3	2.19	0.41
10:Cb:135:ARG:HG3	10:Cb:137:VAL:HG13	2.03	0.41
11:Cd:81:ASN:HA	11:Cd:84:LYS:HG2	2.02	0.41
19:DP:60:ARG:NH1	19:DP:65:ALA:O	2.53	0.41
23:F2:983:LYS:HA	23:F2:983:LYS:HD2	1.85	0.41
24:F3:637:LEU:HD11	24:F3:656:VAL:HG21	2.03	0.41
27:F7:604:ASP:HA	27:F7:607:LYS:HE2	2.03	0.41
32:FE:221:LYS:HE3	32:FE:221:LYS:HB2	1.95	0.41
37:FU:278:MET:SD	37:FU:278:MET:N	2.94	0.41
59:UY:224:UNK:HA	59:UY:227:UNK:HG3	2.03	0.41
1:CE:345:ASP:OD1	1:CE:345:ASP:N	2.54	0.41
4:CK:297:ASP:OD1	4:CK:297:ASP:N	2.53	0.41
9:Ca:368:ARG:NH2	39:FX:14:TYR:O	2.52	0.41
12:Cj:235:PRO:HG3	14:Cp:51:SER:HA	2.03	0.41
24:F3:861:VAL:HG11	24:F3:898:VAL:HG23	2.02	0.41
26:F6:471:ASN:OD1	26:F6:471:ASN:N	2.49	0.41
28:F8:257:HIS:HE1	28:F8:487:LEU:HB3	1.85	0.41
31:FB:173:TYR:OH	33:FJ:362:ARG:O	2.38	0.41
35:FO:298:TRP:CD1	35:FO:299:TYR:H	2.39	0.41
59:UY:251:UNK:CG	59:UY:330:UNK:HG1	2.51	0.41
1:CE:33:MET:O	1:CE:40:ARG:NH2	2.46	0.41
1:CE:395:THR:OG1	1:CE:396:LEU:N	2.53	0.41
2:CF:53:ASP:OD1	2:CF:53:ASP:N	2.48	0.41
15:DD:379:GLN:NE2	21:DU:194:LYS:O	2.54	0.41
16:DI:303:ILE:O	16:DI:314:GLN:NE2	2.53	0.41
19:DP:185:ASP:OD1	19:DP:185:ASP:N	2.50	0.41
23:F2:53:PRO:HB2	23:F2:55:VAL:HG13	2.01	0.41
27:F7:100:ASP:OD2	27:F7:136:LYS:NZ	2.41	0.41
31:FB:373:ALA:HB1	31:FB:484:LEU:HG	2.02	0.41
35:FO:212:LYS:HE3	35:FO:212:LYS:HB2	1.91	0.41
35:FO:295:ARG:HG3	35:FO:308:TYR:HB2	2.01	0.41
37:FS:126:VAL:O	37:FU:208:GLN:NE2	2.46	0.41
37:FU:172:LEU:HD12	37:FU:172:LEU:HA	1.97	0.41
37:FU:240:LEU:HD13	37:FU:240:LEU:HA	1.97	0.41
38:FW:88:CYS:SG	38:FW:89:SER:N	2.94	0.41
59:UY:31:UNK:HG3	59:UY:114:UNK:HB1	2.03	0.41
1:CE:314:MET:HB3	1:CE:324:LEU:HB3	2.03	0.41
2:CF:30:TYR:OH	11:Cd:151:VAL:O	2.30	0.41
5:CO:328:VAL:HG23	15:DD:258:SER:HA	2.02	0.41
9:Ca:123:LYS:HA	9:Ca:126:THR:HG22	2.03	0.41
9:Ca:164:ARG:HH22	50:UP:6:UNK:HG2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Ca:335:ARG:HH22	15:DD:776:ALA:HA	1.86	0.41
11:Cd:67:GLU:HG2	15:DD:156:GLN:HE22	1.86	0.41
16:DI:256:ARG:HH12	24:F3:921:VAL:HG21	1.86	0.41
17:DL:91:PHE:HB2	17:DL:109:VAL:HG11	2.03	0.41
18:DO:198:ARG:HB2	18:DO:255:ARG:HH21	1.85	0.41
20:DR:249:GLU:HB3	20:DR:265:MET:HG3	2.02	0.41
21:DU:15:GLY:O	21:DU:18:GLN:HB2	2.21	0.41
23:F2:941:ARG:HH22	29:F9:51:ASN:HD21	1.69	0.41
24:F3:628:CYS:O	24:F3:663:TYR:OH	2.34	0.41
24:F3:926:SER:OG	24:F3:928:ASP:OD1	2.34	0.41
25:F5:323:GLU:HB3	25:F5:327:ARG:HH21	1.86	0.41
30:FA:195:PRO:HD2	30:FA:198:THR:HG21	2.03	0.41
33:FJ:271:LEU:HB2	33:FJ:276:LYS:HE3	2.02	0.41
34:FN:292:ARG:HD3	34:FN:320:GLU:HB2	2.02	0.41
37:FS:135:MET:HE1	37:FS:142:LYS:HE2	2.03	0.41
37:FS:142:LYS:NZ	37:FS:200:ASP:OD1	2.46	0.41
37:FT:135:MET:HG2	37:FT:144:HIS:HD2	1.84	0.41
40:FY:155:LEU:HA	40:FY:175:PRO:HB3	2.03	0.41
45:Fd:42:HIS:O	45:Fd:46:ARG:NH1	2.54	0.41
1:CE:208:GLN:HB3	1:CE:212:MET:HE3	2.03	0.41
9:Ca:82:PRO:HG2	9:Ca:85:LEU:HD12	2.04	0.41
9:Ca:424:MET:HE3	9:Ca:424:MET:HB2	2.01	0.41
16:DI:30:GLN:H	16:DI:30:GLN:HG2	1.65	0.41
16:DI:227:ASN:OD1	16:DI:231:GLY:N	2.54	0.41
17:DL:125:HIS:HB3	17:DL:197:ALA:HB1	2.03	0.41
24:F3:812:LEU:HB3	24:F3:814:LEU:HD23	2.03	0.41
25:F5:393:PRO:O	25:F5:397:THR:OG1	2.34	0.41
31:FB:539:ARG:NH2	60:CA:232:G:O6	2.54	0.41
31:FB:564:ASP:HA	31:FB:567:ARG:HB2	2.03	0.41
34:FM:226:ASP:HA	34:FM:231:SER:HB3	2.02	0.41
35:FO:98:TYR:OH	60:CA:158:G:OP2	2.30	0.41
5:CO:281:HIS:HB3	27:F7:634:TRP:HB2	2.03	0.40
7:CQ:72:ARG:HD3	15:DD:708:TRP:CD2	2.55	0.40
8:CR:83:TRP:CE2	10:Cb:122:LEU:HB3	2.56	0.40
9:Ca:204:PRO:HG3	9:Ca:257:ILE:HD12	2.03	0.40
16:DI:243:LEU:HD12	16:DI:243:LEU:HA	1.94	0.40
24:F3:326:HIS:ND1	24:F3:375:GLU:OE1	2.46	0.40
25:F5:327:ARG:NH1	25:F5:489:PHE:O	2.54	0.40
28:F8:432:MET:HE3	32:FE:93:ARG:HB2	2.03	0.40
33:FJ:155:LYS:HB3	33:FJ:261:ILE:HG12	2.03	0.40
37:FR:227:THR:HB	37:FS:226:VAL:HG13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:FS:80:ALA:HA	37:FU:250:ARG:HB2	2.03	0.40
43:Fb:144:PRO:HA	43:Fb:145:PRO:HD3	1.97	0.40
59:UY:352:UNK:HG1	60:CA:276:U:O2'	2.21	0.40
2:CF:48:TYR:HA	4:CK:181:MET:HE3	2.02	0.40
15:DD:677:LEU:HD11	36:FP:331:PRO:HA	2.04	0.40
16:DI:277:SER:HB3	24:F3:923:PRO:HG3	2.02	0.40
24:F3:822:VAL:HG21	24:F3:874:LEU:HD13	2.02	0.40
25:F5:380:ASP:OD2	25:F5:384:ARG:NH2	2.55	0.40
28:F8:49:THR:OG1	28:F8:50:THR:N	2.54	0.40
33:FJ:220:PHE:HB3	33:FJ:264:GLY:H	1.85	0.40
37:FQ:194:VAL:HG22	37:FQ:198:THR:HB	2.01	0.40
59:UY:234:UNK:HA	59:UY:237:UNK:HG3	2.03	0.40
1:CE:375:ARG:NH2	16:DI:373:LEU:O	2.55	0.40
8:CR:181:ARG:CZ	26:F6:439:PRO:HB3	2.52	0.40
9:Ca:220:LEU:O	22:DZ:82:LYS:NZ	2.55	0.40
9:Ca:308:LYS:NZ	9:Ca:312:ASP:OD2	2.43	0.40
9:Ca:335:ARG:NH2	15:DD:775:TYR:O	2.55	0.40
15:DD:702:TYR:OH	15:DD:736:TYR:O	2.30	0.40
20:DR:22:LEU:HD22	24:F3:486:ILE:HG23	2.03	0.40
27:F7:47:TRP:CD1	27:F7:285:ARG:HD2	2.55	0.40
32:FE:60:LYS:HG2	32:FE:111:ASP:HB2	2.02	0.40
37:FR:179:CYS:HB2	37:FR:189:PHE:HD1	1.87	0.40
40:FY:160:LEU:HD22	60:CA:344:C:H5''	2.02	0.40
42:Fa:163:HIS:HB2	42:Fa:166:ALA:HB2	2.02	0.40
60:CA:229:G:H1	60:CA:251:U:H3	1.69	0.40
3:CH:180:GLY:HA3	3:CH:262:ILE:HG13	2.04	0.40
18:DO:232:ASN:HB3	27:F7:522:ARG:HH11	1.87	0.40
24:F3:533:SER:HB3	24:F3:574:VAL:HG22	2.03	0.40
27:F7:441:ILE:O	27:F7:445:HIS:HB2	2.22	0.40
59:UY:389:UNK:HG3	59:UY:453:UNK:O	2.22	0.40
2:CF:99:GLU:OE2	5:CO:170:ARG:NH2	2.51	0.40
3:CH:150:THR:HG23	60:CA:319:U:H5	1.86	0.40
8:CR:183:GLN:OE1	42:Fa:59:HIS:NE2	2.54	0.40
10:Cb:54:HIS:HB3	17:DL:147:ILE:HD13	2.04	0.40
22:DZ:90:VAL:HG22	25:F5:687:GLU:HB2	2.04	0.40
24:F3:700:GLY:HA2	24:F3:707:LEU:HD11	2.03	0.40
27:F7:146:THR:HG22	27:F7:148:GLY:H	1.86	0.40
29:F9:32:GLN:N	29:F9:35:GLU:OE1	2.51	0.40
30:FA:152:LEU:HD22	30:FA:178:PHE:HD1	1.86	0.40
35:FO:292:ARG:HE	35:FO:306:ASN:HD22	1.69	0.40
45:Fd:47:LEU:HG	45:Fd:55:ALA:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CE	390/435 (90%)	379 (97%)	9 (2%)	2 (0%)	24	57
2	CF	157/160 (98%)	152 (97%)	5 (3%)	0	100	100
3	CH	216/282 (77%)	210 (97%)	6 (3%)	0	100	100
4	CK	167/326 (51%)	150 (90%)	17 (10%)	0	100	100
5	CO	354/429 (82%)	347 (98%)	7 (2%)	0	100	100
6	CP	178/188 (95%)	170 (96%)	8 (4%)	0	100	100
7	CQ	217/336 (65%)	209 (96%)	8 (4%)	0	100	100
8	CR	149/320 (47%)	143 (96%)	6 (4%)	0	100	100
9	Ca	508/602 (84%)	493 (97%)	15 (3%)	0	100	100
10	Cb	149/311 (48%)	146 (98%)	3 (2%)	0	100	100
11	Cd	183/440 (42%)	182 (100%)	1 (0%)	0	100	100
12	Cj	224/257 (87%)	218 (97%)	6 (3%)	0	100	100
13	Cn	25/250 (10%)	19 (76%)	6 (24%)	0	100	100
14	Cp	176/187 (94%)	172 (98%)	4 (2%)	0	100	100
15	DD	782/812 (96%)	760 (97%)	22 (3%)	0	100	100
16	DI	388/407 (95%)	379 (98%)	9 (2%)	0	100	100
17	DL	199/307 (65%)	193 (97%)	6 (3%)	0	100	100
18	DO	202/282 (72%)	199 (98%)	3 (2%)	0	100	100
19	DP	210/274 (77%)	206 (98%)	4 (2%)	0	100	100
20	DR	250/270 (93%)	240 (96%)	10 (4%)	0	100	100
21	DU	217/228 (95%)	204 (94%)	13 (6%)	0	100	100
22	DZ	28/94 (30%)	27 (96%)	1 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	F2	909/1024 (89%)	890 (98%)	19 (2%)	0	100	100
24	F3	882/966 (91%)	856 (97%)	26 (3%)	0	100	100
25	F5	474/754 (63%)	459 (97%)	14 (3%)	1 (0%)	43	73
26	F6	450/676 (67%)	435 (97%)	15 (3%)	0	100	100
27	F7	658/679 (97%)	615 (94%)	41 (6%)	2 (0%)	36	67
28	F8	493/726 (68%)	476 (97%)	17 (3%)	0	100	100
29	F9	214/608 (35%)	212 (99%)	2 (1%)	0	100	100
30	FA	573/642 (89%)	555 (97%)	18 (3%)	0	100	100
31	FB	373/579 (64%)	365 (98%)	8 (2%)	0	100	100
31	FC	305/579 (53%)	293 (96%)	12 (4%)	0	100	100
32	FE	432/553 (78%)	414 (96%)	18 (4%)	0	100	100
33	FJ	351/362 (97%)	335 (95%)	16 (5%)	0	100	100
34	FM	324/370 (88%)	320 (99%)	4 (1%)	0	100	100
34	FN	317/370 (86%)	310 (98%)	7 (2%)	0	100	100
35	FO	320/334 (96%)	308 (96%)	12 (4%)	0	100	100
36	FP	346/349 (99%)	332 (96%)	13 (4%)	1 (0%)	36	67
37	FQ	255/307 (83%)	250 (98%)	5 (2%)	0	100	100
37	FR	239/307 (78%)	232 (97%)	7 (3%)	0	100	100
37	FS	271/307 (88%)	265 (98%)	6 (2%)	0	100	100
37	FT	229/307 (75%)	224 (98%)	5 (2%)	0	100	100
37	FU	266/307 (87%)	259 (97%)	7 (3%)	0	100	100
38	FW	243/263 (92%)	237 (98%)	6 (2%)	0	100	100
39	FX	218/239 (91%)	212 (97%)	6 (3%)	0	100	100
40	FY	63/188 (34%)	59 (94%)	4 (6%)	0	100	100
41	FZ	129/178 (72%)	123 (95%)	6 (5%)	0	100	100
42	Fa	161/171 (94%)	160 (99%)	1 (1%)	0	100	100
43	Fb	127/151 (84%)	124 (98%)	3 (2%)	0	100	100
44	Fc	82/148 (55%)	81 (99%)	1 (1%)	0	100	100
45	Fd	94/143 (66%)	93 (99%)	1 (1%)	0	100	100
61	F1	54/1041 (5%)	52 (96%)	2 (4%)	0	100	100
62	FF	14/474 (3%)	13 (93%)	1 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	15235/21299 (72%)	14757 (97%)	472 (3%)	6 (0%)	100	100

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	CE	385	PRO
36	FP	85	LYS
1	CE	384	ALA
25	F5	495	MET
27	F7	565	LEU
27	F7	383	ILE

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	CE	325/372 (87%)	317 (98%)	8 (2%)	42	69
2	CF	143/144 (99%)	140 (98%)	3 (2%)	47	71
3	CH	195/246 (79%)	189 (97%)	6 (3%)	35	64
4	CK	147/284 (52%)	140 (95%)	7 (5%)	23	54
5	CO	314/377 (83%)	306 (98%)	8 (2%)	42	69
6	CP	160/168 (95%)	155 (97%)	5 (3%)	35	64
7	CQ	194/297 (65%)	191 (98%)	3 (2%)	57	75
8	CR	130/279 (47%)	125 (96%)	5 (4%)	29	60
9	Ca	449/543 (83%)	438 (98%)	11 (2%)	43	69
10	Cb	132/267 (49%)	125 (95%)	7 (5%)	20	51
11	Cd	168/381 (44%)	167 (99%)	1 (1%)	78	83
12	Cj	193/219 (88%)	188 (97%)	5 (3%)	40	68
13	Cn	22/210 (10%)	22 (100%)	0	100	100
14	Cp	166/175 (95%)	163 (98%)	3 (2%)	51	73
15	DD	691/711 (97%)	683 (99%)	8 (1%)	63	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	DI	350/365 (96%)	347 (99%)	3 (1%)	70	80
17	DL	173/263 (66%)	171 (99%)	2 (1%)	63	78
18	DO	170/229 (74%)	166 (98%)	4 (2%)	43	69
19	DP	191/239 (80%)	190 (100%)	1 (0%)	81	85
20	DR	221/235 (94%)	215 (97%)	6 (3%)	39	67
21	DU	179/201 (89%)	174 (97%)	5 (3%)	38	66
22	DZ	25/84 (30%)	25 (100%)	0	100	100
23	F2	763/867 (88%)	749 (98%)	14 (2%)	51	73
24	F3	748/809 (92%)	724 (97%)	24 (3%)	34	64
25	F5	293/642 (46%)	284 (97%)	9 (3%)	35	64
26	F6	401/590 (68%)	392 (98%)	9 (2%)	45	71
27	F7	554/577 (96%)	540 (98%)	14 (2%)	42	69
28	F8	410/561 (73%)	405 (99%)	5 (1%)	63	78
29	F9	175/504 (35%)	169 (97%)	6 (3%)	32	63
30	FA	477/526 (91%)	459 (96%)	18 (4%)	29	60
31	FB	322/483 (67%)	313 (97%)	9 (3%)	38	66
31	FC	272/483 (56%)	262 (96%)	10 (4%)	30	61
32	FE	386/486 (79%)	378 (98%)	8 (2%)	47	71
33	FJ	314/323 (97%)	305 (97%)	9 (3%)	37	66
34	FM	257/292 (88%)	249 (97%)	8 (3%)	35	64
34	FN	251/292 (86%)	243 (97%)	8 (3%)	34	64
35	FO	281/290 (97%)	273 (97%)	8 (3%)	38	66
36	FP	270/286 (94%)	261 (97%)	9 (3%)	33	63
37	FQ	211/264 (80%)	203 (96%)	8 (4%)	29	60
37	FR	206/264 (78%)	201 (98%)	5 (2%)	43	69
37	FS	238/264 (90%)	231 (97%)	7 (3%)	37	66
37	FT	200/264 (76%)	192 (96%)	8 (4%)	28	60
37	FU	222/264 (84%)	213 (96%)	9 (4%)	27	59
38	FW	223/234 (95%)	223 (100%)	0	100	100
39	FX	178/195 (91%)	176 (99%)	2 (1%)	65	78
40	FY	61/163 (37%)	58 (95%)	3 (5%)	22	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	FZ	86/156 (55%)	84 (98%)	2 (2%)	44	70
42	Fa	141/149 (95%)	135 (96%)	6 (4%)	26	57
43	Fb	117/135 (87%)	116 (99%)	1 (1%)	70	80
44	Fc	78/127 (61%)	74 (95%)	4 (5%)	21	52
45	Fd	79/119 (66%)	78 (99%)	1 (1%)	61	77
61	F1	46/895 (5%)	44 (96%)	2 (4%)	26	57
62	FF	16/400 (4%)	16 (100%)	0	100	100
All	All	13014/18193 (72%)	12687 (98%)	327 (2%)	42	69

All (327) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CE	204	VAL
1	CE	222	VAL
1	CE	224	VAL
1	CE	225	LEU
1	CE	232	ILE
1	CE	233	VAL
1	CE	330	VAL
1	CE	406	THR
2	CF	39	ILE
2	CF	111	LEU
2	CF	152	THR
3	CH	86	THR
3	CH	90	ASP
3	CH	128	VAL
3	CH	219	ILE
3	CH	257	THR
3	CH	259	ASP
4	CK	144	VAL
4	CK	189	THR
4	CK	207	VAL
4	CK	217	LEU
4	CK	281	VAL
4	CK	295	VAL
4	CK	310	ILE
5	CO	122	VAL
5	CO	162	THR
5	CO	175	VAL
5	CO	178	LEU

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Mol	Chain	Res	Type
5	CO	283	VAL
5	CO	311	ILE
5	CO	367	LEU
5	CO	419	VAL
6	CP	77	SER
6	CP	82	VAL
6	CP	172	VAL
6	CP	184	VAL
6	CP	188	LEU
7	CQ	95	ILE
7	CQ	198	LEU
7	CQ	200	LEU
8	CR	80	LEU
8	CR	131	THR
8	CR	139	THR
8	CR	151	ASN
8	CR	228	VAL
9	Ca	106	ASN
9	Ca	147	VAL
9	Ca	171	THR
9	Ca	187	ASP
9	Ca	243	THR
9	Ca	379	MET
9	Ca	414	THR
9	Ca	449	VAL
9	Ca	456	LEU
9	Ca	574	VAL
9	Ca	579	VAL
10	Cb	28	TYR
10	Cb	96	ASP
10	Cb	137	VAL
10	Cb	146	VAL
10	Cb	182	VAL
10	Cb	184	LEU
10	Cb	195	LEU
11	Cd	33	THR
12	Cj	47	VAL
12	Cj	156	THR
12	Cj	161	VAL
12	Cj	168	VAL
12	Cj	234	THR
14	Cp	12	THR

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Mol	Chain	Res	Type
14	Cp	53	VAL
14	Cp	135	THR
15	DD	211	THR
15	DD	218	VAL
15	DD	410	THR
15	DD	586	VAL
15	DD	653	PHE
15	DD	673	VAL
15	DD	743	LEU
15	DD	754	THR
16	DI	113	VAL
16	DI	198	ASP
16	DI	391	ASP
17	DL	98	ASP
17	DL	243	LEU
18	DO	62	LEU
18	DO	122	LEU
18	DO	127	LEU
18	DO	135	THR
19	DP	88	THR
20	DR	33	VAL
20	DR	90	ASP
20	DR	117	ILE
20	DR	118	VAL
20	DR	190	LEU
20	DR	254	VAL
21	DU	42	THR
21	DU	90	VAL
21	DU	146	THR
21	DU	172	ASP
21	DU	188	VAL
23	F2	28	THR
23	F2	46	THR
23	F2	81	ILE
23	F2	110	GLU
23	F2	313	VAL
23	F2	377	LEU
23	F2	406	VAL
23	F2	460	GLU
23	F2	478	VAL
23	F2	555	LEU
23	F2	768	LEU

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Mol	Chain	Res	Type
23	F2	878	SER
23	F2	948	THR
23	F2	974	VAL
24	F3	112	VAL
24	F3	152	THR
24	F3	180	ILE
24	F3	305	ASP
24	F3	306	VAL
24	F3	374	VAL
24	F3	418	ASP
24	F3	550	THR
24	F3	646	THR
24	F3	660	VAL
24	F3	695	LEU
24	F3	710	LEU
24	F3	720	ILE
24	F3	791	ILE
24	F3	799	ASP
24	F3	810	THR
24	F3	814	LEU
24	F3	833	LEU
24	F3	842	VAL
24	F3	845	ASP
24	F3	861	VAL
24	F3	868	VAL
24	F3	870	ILE
24	F3	940	VAL
25	F5	363	THR
25	F5	379	VAL
25	F5	397	THR
25	F5	403	LEU
25	F5	410	ASP
25	F5	444	VAL
25	F5	597	ARG
25	F5	688	LEU
25	F5	701	LEU
26	F6	192	VAL
26	F6	218	SER
26	F6	220	LEU
26	F6	226	LEU
26	F6	253	SER
26	F6	268	THR

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Mol	Chain	Res	Type
26	F6	323	LEU
26	F6	341	LEU
26	F6	354	THR
27	F7	128	ASP
27	F7	134	VAL
27	F7	202	THR
27	F7	204	ILE
27	F7	207	VAL
27	F7	284	LEU
27	F7	299	SER
27	F7	497	SER
27	F7	532	THR
27	F7	555	THR
27	F7	564	LEU
27	F7	632	THR
27	F7	658	LEU
27	F7	660	VAL
28	F8	50	THR
28	F8	160	VAL
28	F8	165	VAL
28	F8	428	VAL
28	F8	538	VAL
29	F9	19	LEU
29	F9	83	LYS
29	F9	192	LEU
29	F9	201	VAL
29	F9	210	GLN
29	F9	221	ASP
30	FA	51	THR
30	FA	95	VAL
30	FA	161	CYS
30	FA	196	VAL
30	FA	231	VAL
30	FA	232	VAL
30	FA	239	VAL
30	FA	241	LEU
30	FA	250	LEU
30	FA	291	VAL
30	FA	335	LEU
30	FA	378	VAL
30	FA	398	ASP
30	FA	404	LEU

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Mol	Chain	Res	Type
30	FA	408	ILE
30	FA	440	ASP
30	FA	472	LEU
30	FA	626	LEU
31	FB	172	LEU
31	FB	266	VAL
31	FB	278	VAL
31	FB	287	VAL
31	FB	413	ASN
31	FB	450	THR
31	FB	459	VAL
31	FB	471	VAL
31	FB	524	ASP
31	FC	191	VAL
31	FC	254	GLU
31	FC	287	VAL
31	FC	367	ASP
31	FC	477	THR
31	FC	480	THR
31	FC	481	VAL
31	FC	491	ASP
31	FC	495	ILE
31	FC	525	LEU
32	FE	204	GLU
32	FE	241	LEU
32	FE	299	ILE
32	FE	301	VAL
32	FE	353	THR
32	FE	355	VAL
32	FE	392	THR
32	FE	396	THR
33	FJ	85	THR
33	FJ	88	LEU
33	FJ	115	THR
33	FJ	153	ILE
33	FJ	159	LEU
33	FJ	185	LEU
33	FJ	217	ILE
33	FJ	290	LEU
33	FJ	297	LEU
34	FM	114	THR
34	FM	175	ASN

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Mol	Chain	Res	Type
34	FM	207	LEU
34	FM	226	ASP
34	FM	255	THR
34	FM	286	VAL
34	FM	309	SER
34	FM	310	VAL
34	FN	12	VAL
34	FN	56	ASP
34	FN	70	THR
34	FN	92	LEU
34	FN	140	SER
34	FN	258	VAL
34	FN	286	VAL
34	FN	291	LEU
35	FO	75	VAL
35	FO	142	VAL
35	FO	274	VAL
35	FO	284	GLU
35	FO	293	VAL
35	FO	304	ILE
35	FO	326	THR
35	FO	328	ILE
36	FP	115	VAL
36	FP	176	THR
36	FP	182	VAL
36	FP	255	THR
36	FP	256	VAL
36	FP	298	VAL
36	FP	303	LEU
36	FP	315	VAL
36	FP	328	ASP
37	FQ	23	THR
37	FQ	60	THR
37	FQ	107	VAL
37	FQ	128	VAL
37	FQ	190	VAL
37	FQ	191	THR
37	FQ	198	THR
37	FQ	214	THR
37	FR	27	THR
37	FR	58	ASP
37	FR	120	VAL

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Mol	Chain	Res	Type
37	FR	190	VAL
37	FR	214	THR
37	FS	90	VAL
37	FS	98	LEU
37	FS	121	VAL
37	FS	201	LEU
37	FS	214	THR
37	FS	232	VAL
37	FS	305	THR
37	FT	22	GLU
37	FT	107	VAL
37	FT	141	VAL
37	FT	190	VAL
37	FT	192	THR
37	FT	204	THR
37	FT	221	LEU
37	FT	227	THR
37	FU	42	LEU
37	FU	71	LEU
37	FU	73	THR
37	FU	190	VAL
37	FU	191	THR
37	FU	198	THR
37	FU	233	VAL
37	FU	240	LEU
37	FU	253	GLU
39	FX	10	VAL
39	FX	73	THR
40	FY	132	ASP
40	FY	135	GLU
40	FY	177	ILE
41	FZ	32	LEU
41	FZ	43	LEU
42	Fa	27	VAL
42	Fa	76	THR
42	Fa	120	VAL
42	Fa	129	LEU
42	Fa	156	VAL
42	Fa	167	LEU
43	Fb	134	GLN
44	Fc	91	VAL
44	Fc	121	LEU

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Mol	Chain	Res	Type
44	Fc	131	ILE
44	Fc	136	ASP
45	Fd	77	VAL
61	F1	986	GLU
61	F1	1026	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (254) such sidechains are listed below:

Mol	Chain	Res	Type
1	CE	187	GLN
1	CE	317	HIS
1	CE	333	ASN
2	CF	86	HIS
3	CH	29	HIS
3	CH	54	GLN
3	CH	55	GLN
3	CH	111	GLN
3	CH	188	HIS
3	CH	198	HIS
3	CH	247	HIS
3	CH	282	HIS
4	CK	286	ASN
4	CK	289	GLN
4	CK	316	ASN
5	CO	98	ASN
5	CO	111	GLN
5	CO	135	GLN
5	CO	197	GLN
5	CO	246	ASN
5	CO	297	GLN
5	CO	325	ASN
5	CO	350	HIS
5	CO	356	GLN
6	CP	19	GLN
7	CQ	20	GLN
7	CQ	36	ASN
7	CQ	38	ASN
7	CQ	49	ASN
7	CQ	122	GLN
7	CQ	158	HIS
8	CR	65	GLN
8	CR	183	GLN

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Mol	Chain	Res	Type
8	CR	191	GLN
8	CR	211	ASN
8	CR	214	GLN
8	CR	229	HIS
9	Ca	106	ASN
9	Ca	223	ASN
9	Ca	227	ASN
9	Ca	339	HIS
10	Cb	191	HIS
11	Cd	72	ASN
11	Cd	87	GLN
11	Cd	98	GLN
11	Cd	113	GLN
11	Cd	119	HIS
11	Cd	159	HIS
11	Cd	192	ASN
13	Cn	156	ASN
14	Cp	37	GLN
14	Cp	55	ASN
14	Cp	113	GLN
14	Cp	169	ASN
15	DD	45	GLN
15	DD	63	GLN
15	DD	64	HIS
15	DD	82	ASN
15	DD	144	ASN
15	DD	156	GLN
15	DD	273	HIS
15	DD	276	HIS
15	DD	300	GLN
15	DD	353	HIS
15	DD	387	GLN
15	DD	402	GLN
15	DD	408	HIS
15	DD	453	ASN
15	DD	499	ASN
15	DD	542	HIS
15	DD	669	HIS
15	DD	687	HIS
15	DD	798	HIS
16	DI	18	HIS
16	DI	30	GLN

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Mol	Chain	Res	Type
16	DI	175	GLN
16	DI	320	GLN
16	DI	370	GLN
16	DI	372	ASN
17	DL	132	ASN
17	DL	182	GLN
18	DO	71	HIS
18	DO	148	ASN
18	DO	159	HIS
18	DO	197	GLN
19	DP	36	GLN
19	DP	116	HIS
19	DP	143	ASN
20	DR	68	HIS
20	DR	162	GLN
20	DR	173	ASN
20	DR	268	HIS
21	DU	19	GLN
21	DU	58	HIS
22	DZ	73	HIS
23	F2	219	GLN
23	F2	307	ASN
23	F2	337	GLN
23	F2	461	HIS
23	F2	635	GLN
23	F2	844	ASN
23	F2	958	ASN
24	F3	79	HIS
24	F3	265	HIS
24	F3	321	ASN
24	F3	405	ASN
24	F3	432	GLN
24	F3	475	ASN
24	F3	481	HIS
24	F3	530	HIS
24	F3	588	HIS
24	F3	650	GLN
24	F3	654	GLN
24	F3	747	HIS
24	F3	796	ASN
24	F3	905	HIS
25	F5	320	GLN

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Mol	Chain	Res	Type
25	F5	401	GLN
25	F5	609	GLN
25	F5	753	ASN
26	F6	7	HIS
26	F6	25	GLN
26	F6	203	GLN
26	F6	210	GLN
26	F6	251	GLN
26	F6	319	HIS
26	F6	385	GLN
27	F7	61	HIS
27	F7	93	HIS
27	F7	109	ASN
27	F7	157	GLN
27	F7	173	GLN
27	F7	232	ASN
27	F7	283	ASN
27	F7	445	HIS
27	F7	542	ASN
28	F8	68	HIS
28	F8	179	HIS
28	F8	219	HIS
28	F8	244	HIS
28	F8	257	HIS
28	F8	696	GLN
29	F9	32	GLN
29	F9	51	ASN
29	F9	132	GLN
29	F9	212	HIS
30	FA	147	ASN
30	FA	181	GLN
30	FA	326	ASN
30	FA	534	ASN
30	FA	561	ASN
31	FB	192	GLN
31	FB	194	GLN
31	FB	248	HIS
31	FB	329	HIS
31	FB	363	HIS
31	FB	392	ASN
31	FB	413	ASN
31	FB	441	ASN

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Mol	Chain	Res	Type
31	FB	464	HIS
31	FB	489	GLN
31	FB	529	GLN
31	FC	312	GLN
31	FC	326	GLN
31	FC	345	ASN
31	FC	474	ASN
31	FC	489	GLN
31	FC	505	HIS
31	FC	519	HIS
31	FC	565	GLN
31	FC	566	HIS
32	FE	119	ASN
32	FE	126	ASN
32	FE	136	GLN
32	FE	155	HIS
32	FE	165	GLN
32	FE	242	ASN
32	FE	438	GLN
33	FJ	35	GLN
33	FJ	41	HIS
33	FJ	89	GLN
33	FJ	195	HIS
33	FJ	235	HIS
33	FJ	236	GLN
33	FJ	238	ASN
34	FM	96	ASN
34	FM	102	ASN
34	FM	125	HIS
34	FM	211	HIS
34	FM	243	GLN
34	FN	9	ASN
34	FN	17	ASN
34	FN	25	ASN
34	FN	102	ASN
34	FN	312	HIS
34	FN	323	ASN
35	FO	46	HIS
35	FO	94	HIS
35	FO	111	HIS
35	FO	135	ASN
35	FO	147	ASN

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Mol	Chain	Res	Type
35	FO	151	GLN
35	FO	157	GLN
35	FO	181	ASN
35	FO	265	ASN
35	FO	318	GLN
36	FP	31	GLN
36	FP	116	GLN
36	FP	120	ASN
37	FQ	15	ASN
37	FQ	74	ASN
37	FQ	82	ASN
37	FQ	101	HIS
37	FQ	139	GLN
37	FQ	178	GLN
37	FQ	209	GLN
37	FQ	234	HIS
37	FR	38	GLN
37	FR	75	GLN
37	FR	94	ASN
37	FR	130	GLN
37	FR	171	GLN
37	FR	213	HIS
37	FR	243	ASN
37	FS	15	ASN
37	FS	178	GLN
37	FS	213	HIS
37	FS	234	HIS
37	FS	243	ASN
37	FT	38	GLN
37	FT	74	ASN
37	FU	29	HIS
37	FU	144	HIS
37	FU	171	GLN
37	FU	213	HIS
38	FW	20	GLN
38	FW	77	GLN
38	FW	178	HIS
38	FW	246	HIS
39	FX	38	ASN
39	FX	68	GLN
39	FX	154	GLN
39	FX	164	HIS

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Mol	Chain	Res	Type
39	FX	168	HIS
40	FY	165	GLN
40	FY	166	HIS
41	FZ	53	HIS
41	FZ	69	ASN
41	FZ	170	ASN
42	Fa	126	GLN
43	Fb	134	GLN
44	Fc	96	HIS
45	Fd	76	HIS
61	F1	1006	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
60	CA	459/474 (96%)	190 (41%)	6 (1%)

All (190) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
60	CA	3	A
60	CA	4	A
60	CA	5	U
60	CA	6	U
60	CA	7	A
60	CA	10	G
60	CA	17	G
60	CA	21	G
60	CA	22	U
60	CA	26	C
60	CA	27	A
60	CA	29	A
60	CA	30	U
60	CA	32	A
60	CA	35	U
60	CA	36	U
60	CA	39	U
60	CA	44	U
60	CA	46	U
60	CA	48	U
60	CA	49	U

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Mol	Chain	Res	Type
60	CA	50	A
60	CA	53	A
60	CA	58	A
60	CA	60	A
60	CA	67	U
60	CA	72	U
60	CA	73	U
60	CA	74	G
60	CA	78	G
60	CA	79	A
60	CA	80	U
60	CA	81	U
60	CA	82	U
60	CA	84	U
60	CA	85	U
60	CA	86	G
60	CA	87	U
60	CA	88	A
60	CA	90	A
60	CA	95	U
60	CA	97	U
60	CA	98	A
60	CA	100	G
60	CA	102	A
60	CA	105	G
60	CA	106	U
60	CA	111	A
60	CA	112	A
60	CA	113	U
60	CA	115	A
60	CA	127	G
60	CA	135	U
60	CA	136	G
60	CA	137	U
60	CA	138	U
60	CA	139	U
60	CA	140	U
60	CA	152	U
60	CA	153	A
60	CA	154	G
60	CA	155	A
60	CA	157	G

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Mol	Chain	Res	Type
60	CA	159	G
60	CA	160	U
60	CA	161	G
60	CA	167	A
60	CA	169	A
60	CA	170	U
60	CA	172	A
60	CA	173	A
60	CA	174	A
60	CA	178	A
60	CA	179	U
60	CA	181	A
60	CA	182	U
60	CA	185	A
60	CA	190	U
60	CA	191	A
60	CA	192	U
60	CA	195	A
60	CA	196	U
60	CA	197	A
60	CA	198	A
60	CA	205	A
60	CA	207	A
60	CA	208	U
60	CA	214	U
60	CA	217	U
60	CA	218	A
60	CA	219	G
60	CA	220	U
60	CA	221	C
60	CA	223	G
60	CA	227	U
60	CA	228	G
60	CA	232	G
60	CA	236	G
60	CA	238	C
60	CA	239	G
60	CA	240	U
60	CA	241	U
60	CA	242	G
60	CA	247	A
60	CA	249	U

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Mol	Chain	Res	Type
60	CA	253	U
60	CA	256	G
60	CA	257	C
60	CA	258	U
60	CA	259	U
60	CA	260	U
60	CA	261	U
60	CA	262	A
60	CA	267	U
60	CA	268	U
60	CA	269	A
60	CA	270	U
60	CA	271	A
60	CA	272	C
60	CA	278	U
60	CA	281	U
60	CA	282	A
60	CA	283	U
60	CA	284	U
60	CA	285	A
60	CA	286	A
60	CA	291	U
60	CA	292	U
60	CA	293	A
60	CA	294	A
60	CA	296	U
60	CA	297	G
60	CA	298	C
60	CA	299	U
60	CA	304	U
60	CA	306	A
60	CA	318	A
60	CA	320	A
60	CA	321	A
60	CA	322	A
60	CA	323	U
60	CA	324	A
60	CA	327	U
60	CA	330	U
60	CA	337	U
60	CA	338	U
60	CA	339	U

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Mol	Chain	Res	Type
60	CA	340	U
60	CA	341	A
60	CA	347	C
60	CA	350	U
60	CA	351	A
60	CA	353	G
60	CA	355	A
60	CA	357	A
60	CA	359	G
60	CA	366	U
60	CA	367	A
60	CA	368	A
60	CA	370	A
60	CA	375	A
60	CA	377	U
60	CA	378	A
60	CA	381	U
60	CA	532	A
60	CA	533	A
60	CA	534	A
60	CA	538	A
60	CA	539	A
60	CA	540	A
60	CA	558	A
60	CA	559	A
60	CA	560	U
60	CA	565	A
60	CA	576	A
60	CA	577	A
60	CA	579	G
60	CA	581	G
60	CA	582	C
60	CA	587	A
60	CA	590	A
60	CA	599	A
60	CA	600	U
60	CA	601	A
60	CA	602	A
60	CA	603	A
60	CA	613	U
60	CA	616	U
60	CA	617	U

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Mol	Chain	Res	Type
60	CA	619	U

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
60	CA	78	G
60	CA	160	U
60	CA	173	A
60	CA	285	A
60	CA	296	U
60	CA	349	U

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	$\# Z > 2$
60	UBD	CA	620	60	22,25,26	0.64	0	32,37,40	0.63	1 (3%)

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
60	UBD	CA	620	60	-	1/12/30/31	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	CA	620	UBD	O6P-P2-O5P	2.20	119.41	110.83

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	CA	620	UBD	O4'-C4'-C5'-O5'

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 7 ligands modelled in this entry, 5 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
65	PM8	FcA	1	44	26,31,31	0.71	1 (3%)	30,38,38	0.92	1 (3%)
64	PO4	FWA	1	-	4,4,4	1.02	0	6,6,6	0.48	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
65	PM8	FcA	1	44	-	2/36/38/38	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
65	FcA	1	PM8	C2-C1	2.39	1.53	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
65	FcA	1	PM8	O1-C1-C2	-2.41	121.19	123.98

There are no chirality outliers.

All (2) torsion outliers are listed below:

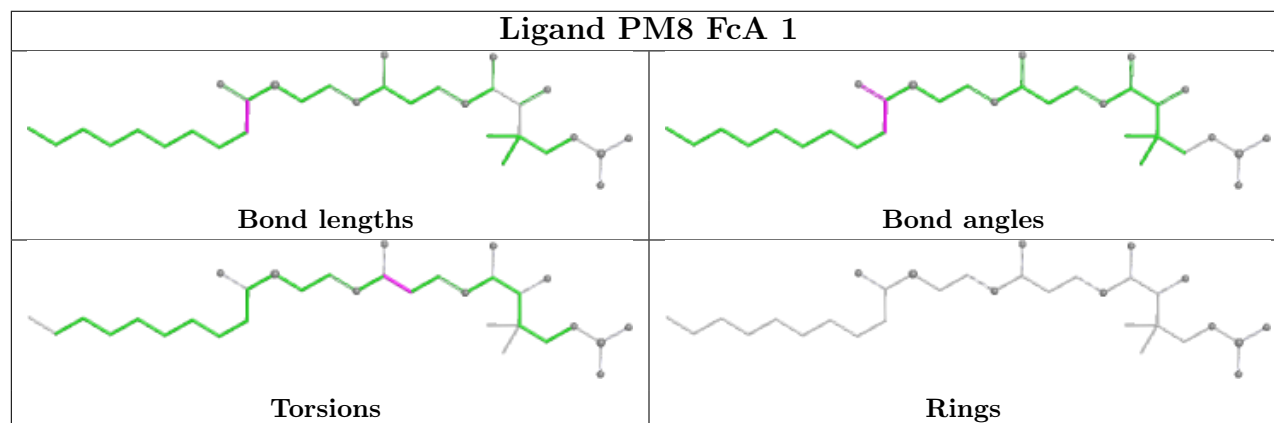
Mol	Chain	Res	Type	Atoms
65	FcA	1	PM8	C37-C38-C39-O40
65	FcA	1	PM8	C37-C38-C39-N41

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
65	FcA	1	PM8	1	0
64	FWA	1	PO4	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
59	UY	13
47	UB	2
60	CA	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	UY	347:UNK	C	348:UNK	N	76.88
1	UY	439:UNK	C	440:UNK	N	65.92
1	UB	10:UNK	C	101:UNK	N	45.41
1	UY	338:UNK	C	339:UNK	N	40.51
1	UY	411:UNK	C	412:UNK	N	35.07
1	UB	110:UNK	C	201:UNK	N	25.42
1	UY	455:UNK	C	456:UNK	N	20.24
1	UY	394:UNK	C	395:UNK	N	15.52
1	CA	383:U	O3'	530:A	P	14.05
1	UY	430:UNK	C	431:UNK	N	11.78
1	UY	245:UNK	C	246:UNK	N	6.90
1	UY	403:UNK	C	405:UNK	N	6.75
1	UY	125:UNK	C	126:UNK	N	5.66
1	UY	117:UNK	C	118:UNK	N	5.52
1	UY	426:UNK	C	427:UNK	N	4.10
1	UY	56:UNK	C	57:UNK	N	3.43

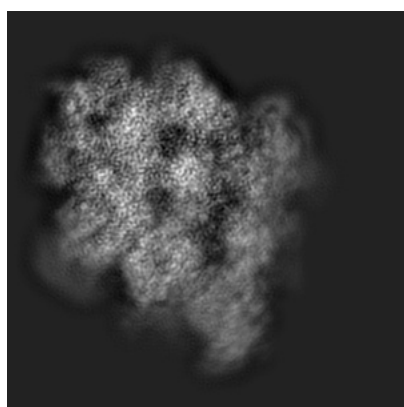
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10177. These allow visual inspection of the internal detail of the map and identification of artifacts.

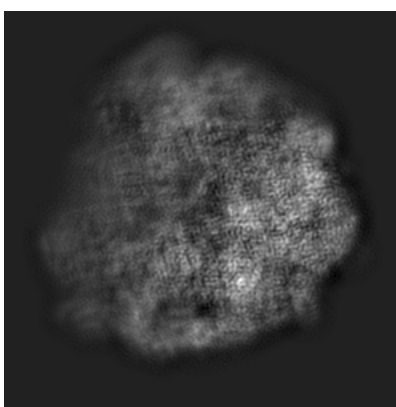
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

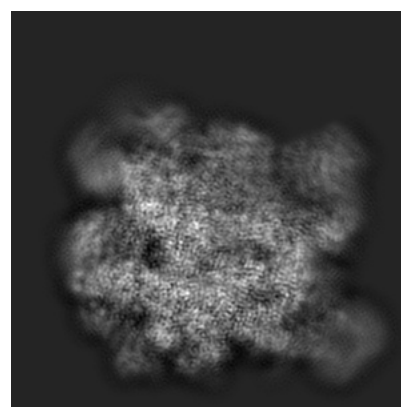
6.1.1 Primary map



X



Y

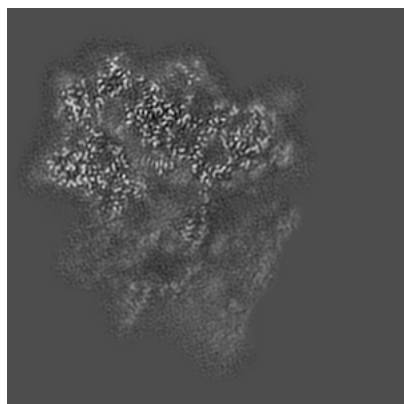


Z

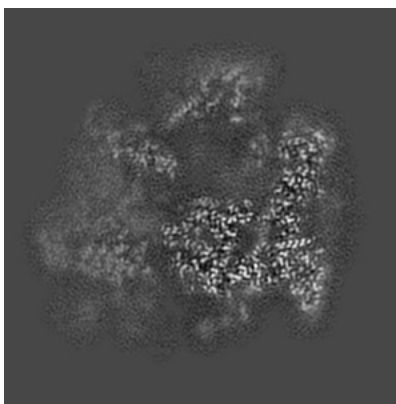
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

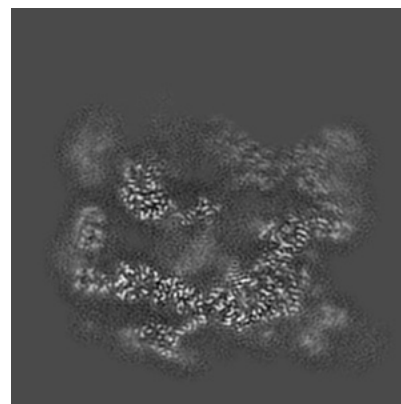
6.2.1 Primary map



X Index: 120



Y Index: 120

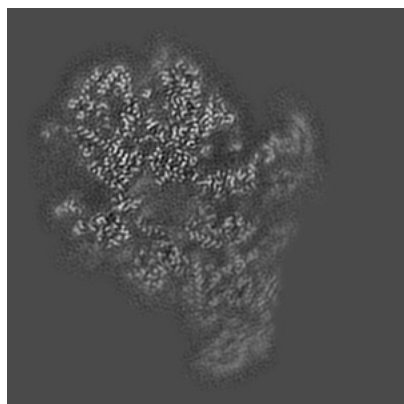


Z Index: 120

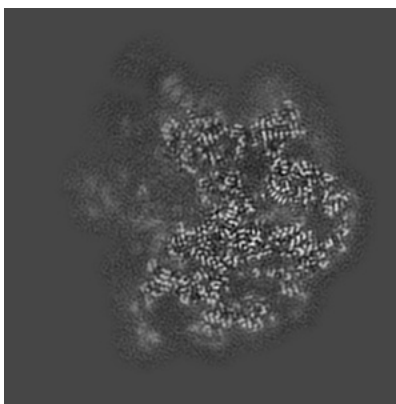
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

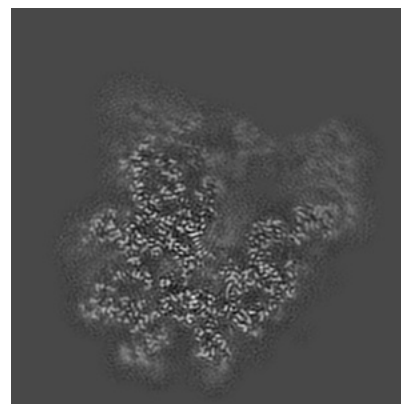
6.3.1 Primary map



X Index: 98



Y Index: 70

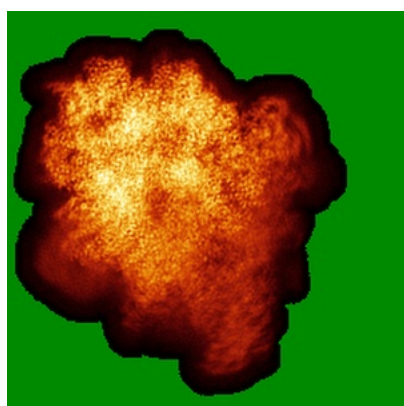


Z Index: 140

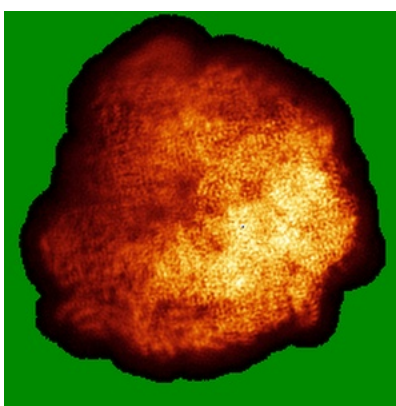
The images above show the largest variance slices of the map in three orthogonal directions.

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

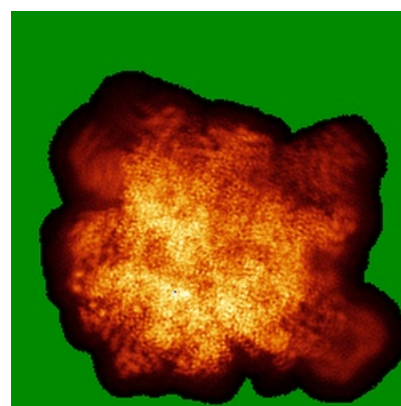
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

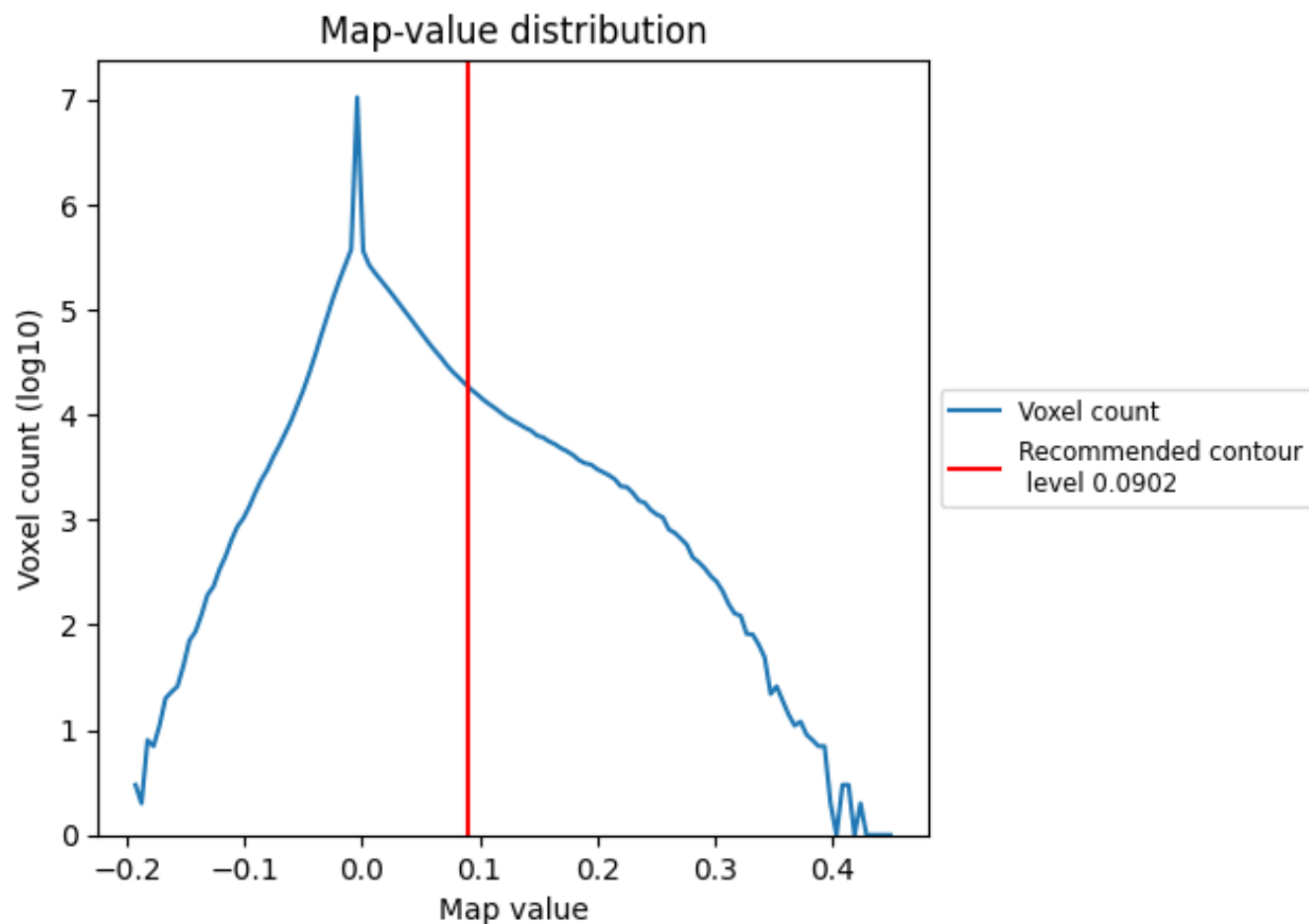
6.6 Mask visualisation

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

7 Map analysis [i](#)

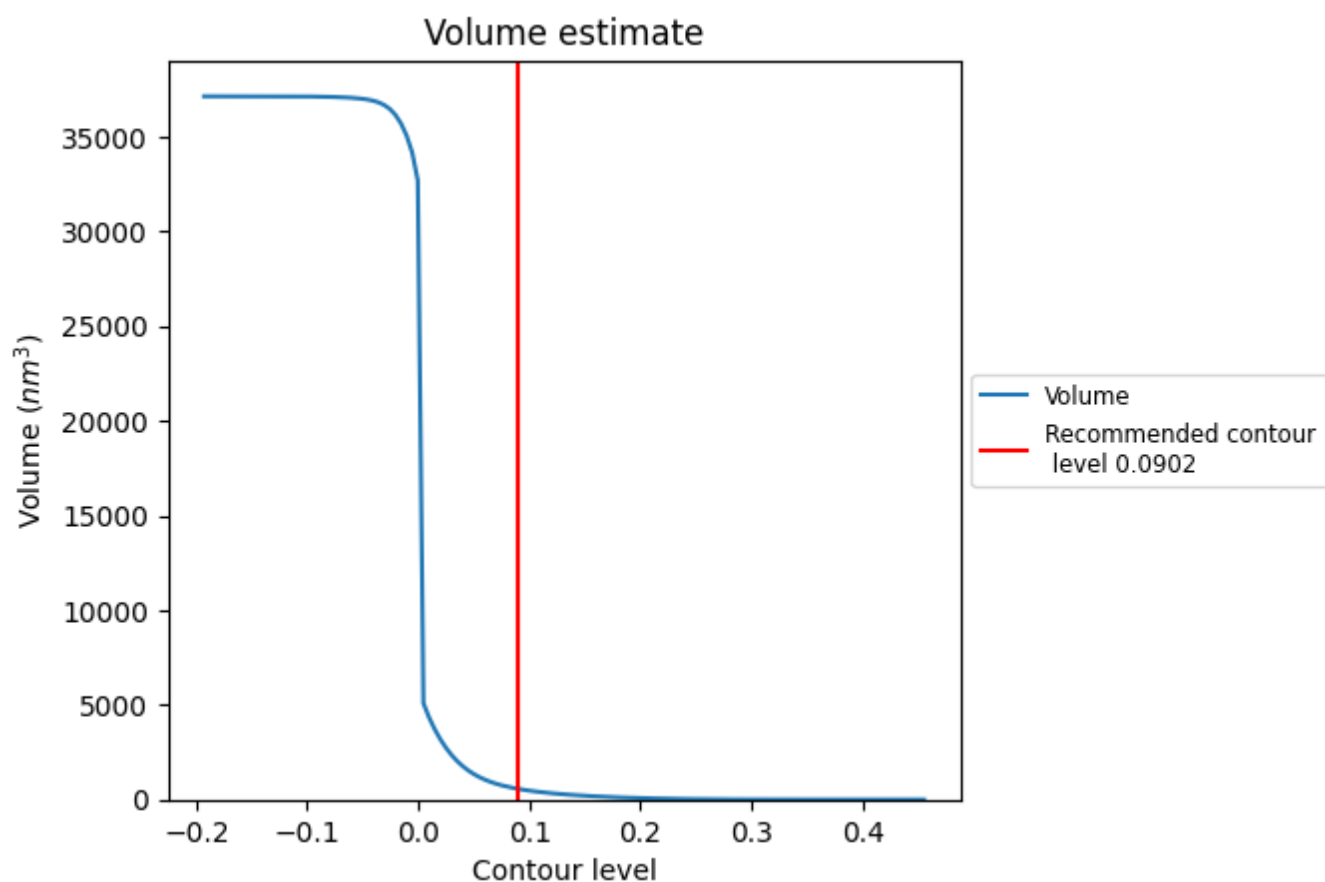
This section contains the results of statistical analysis of the map.

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.

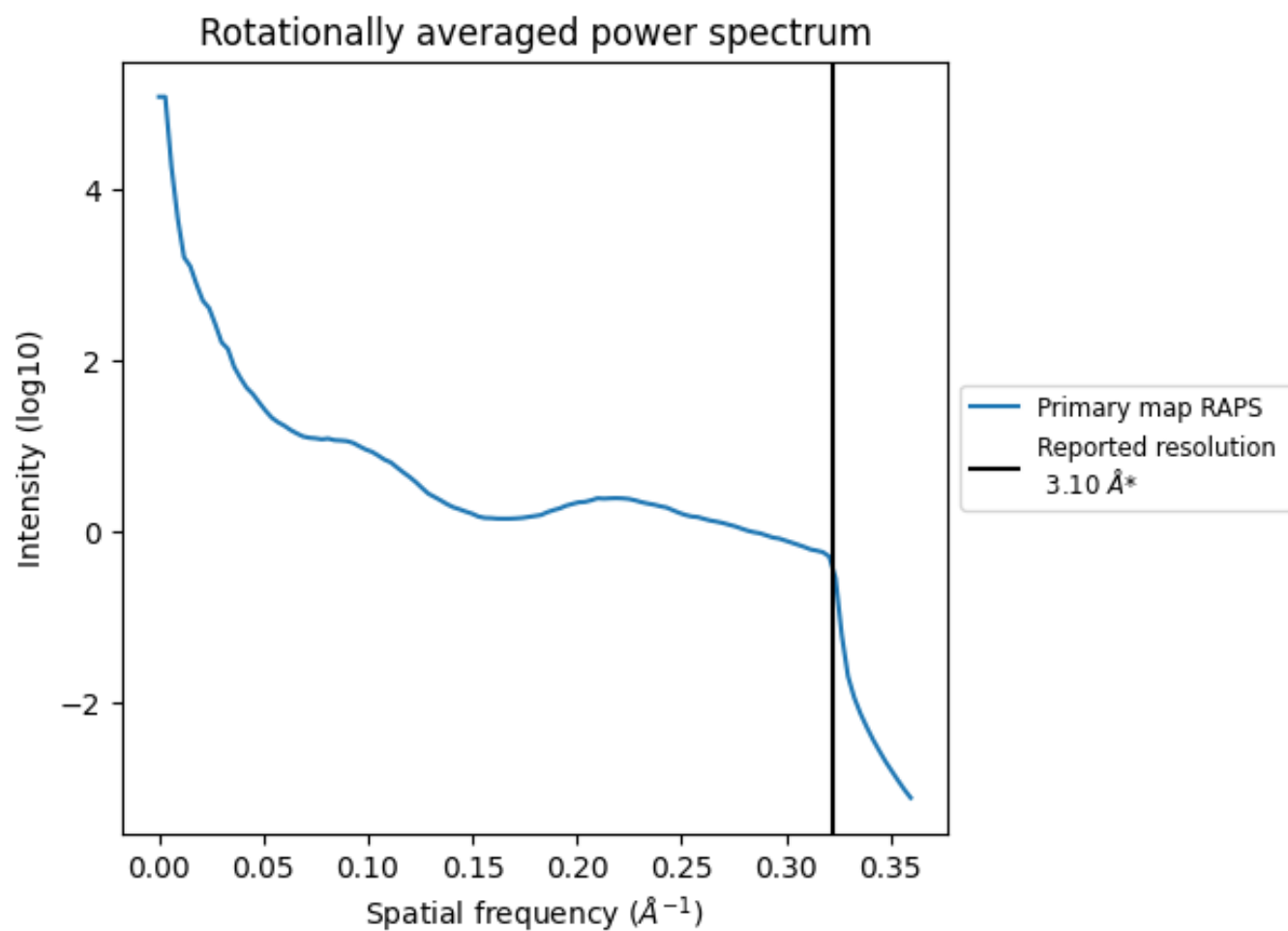
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 560 nm³; this corresponds to an approximate mass of 505 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 0.323 Å⁻¹

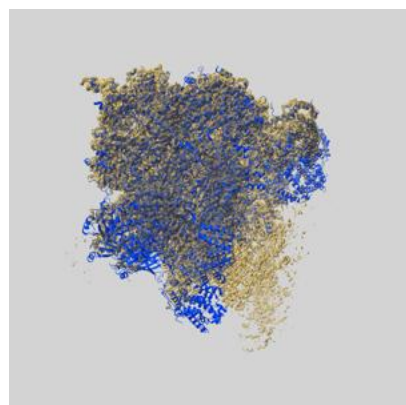
8 Fourier-Shell correlation

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

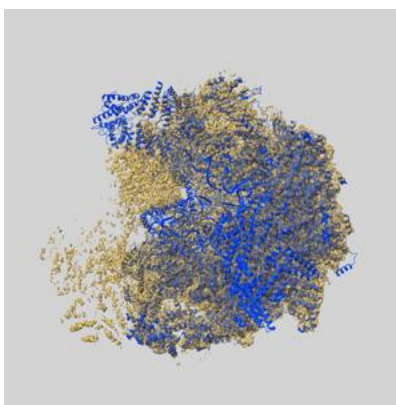
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10177 and PDB model 6SGA. Per-residue inclusion information can be found in section 3 on page 19.

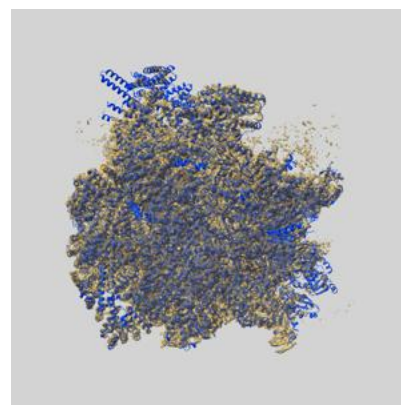
9.1 Map-model overlay [i](#)



X



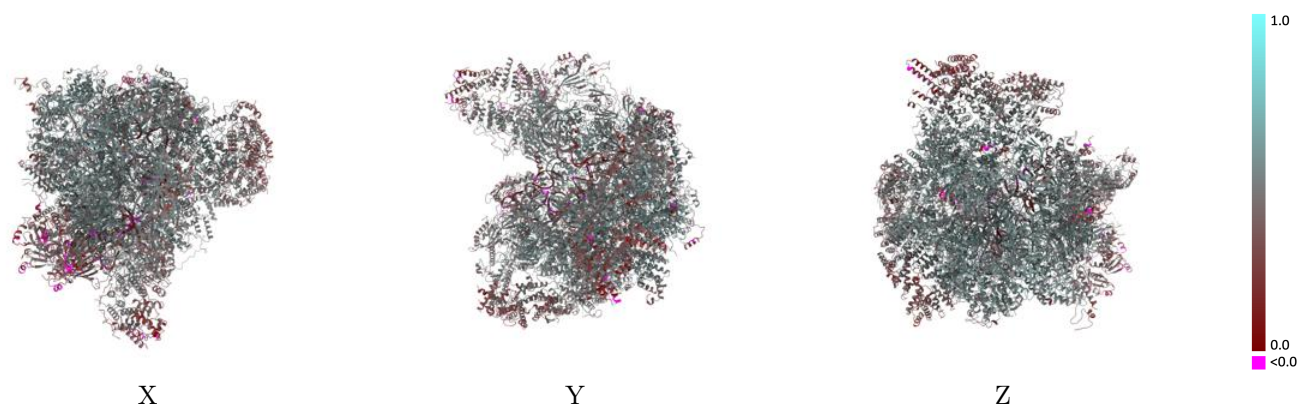
Y



Z

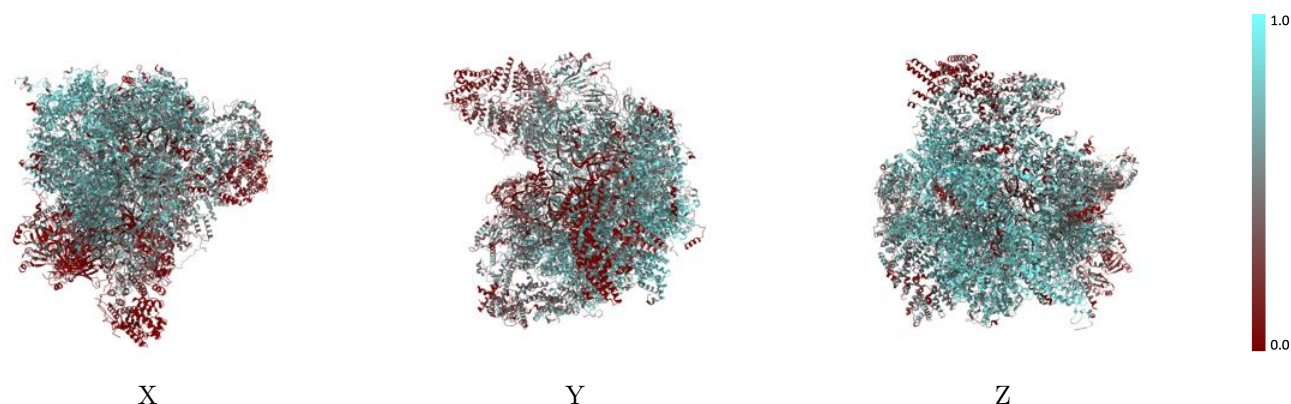
The images above show the 3D surface view of the map at the recommended contour level 0.0902 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



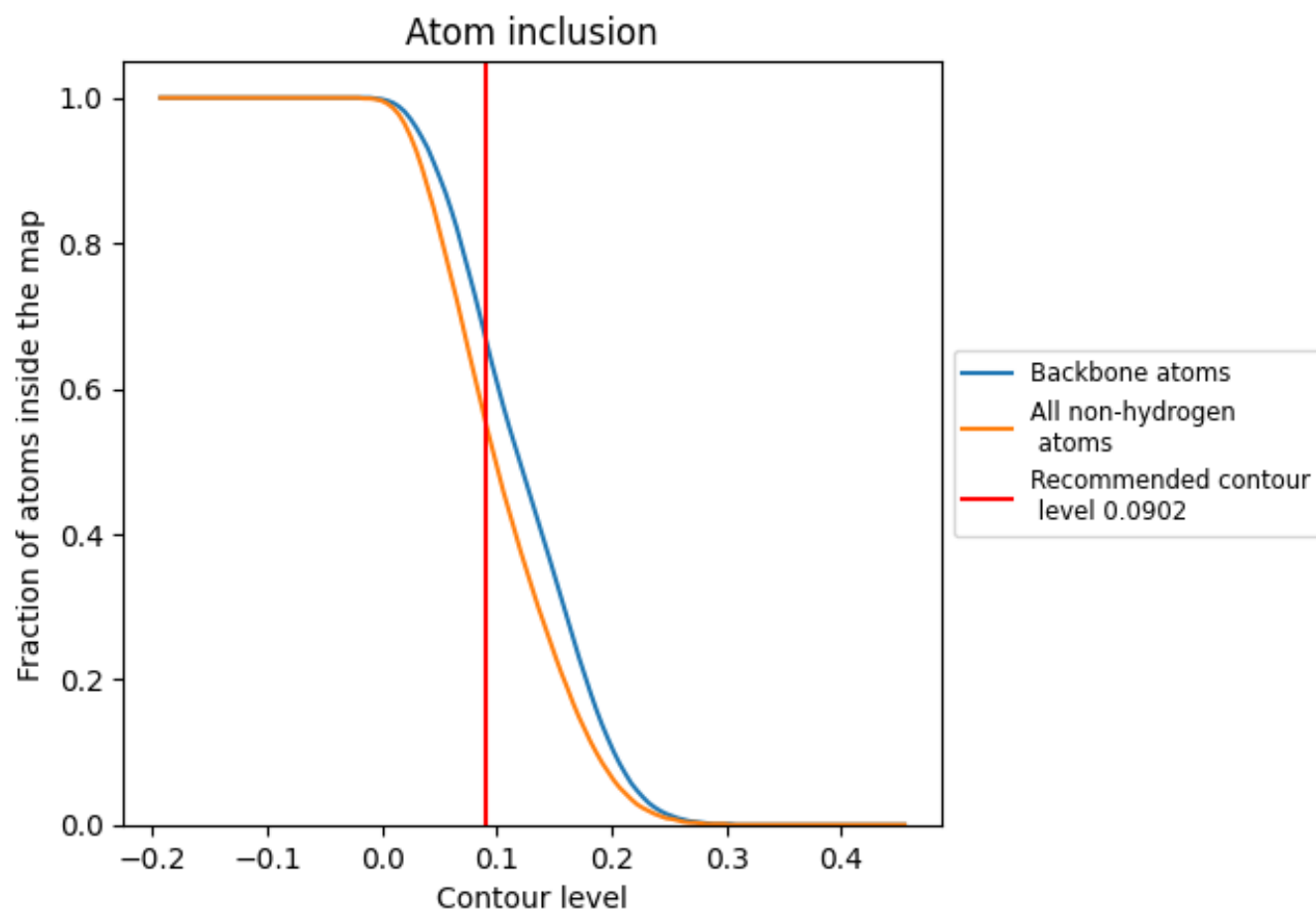
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0902).

9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 55% 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 (0.0902) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5540	 0.4790
CA	 0.5250	 0.4310
CAA	 1.0000	 0.7430
CAB	 1.0000	 0.7010
CE	 0.6110	 0.5220
CF	 0.6600	 0.5140
CH	 0.6880	 0.5500
CK	 0.4290	 0.4490
CO	 0.7080	 0.5420
CP	 0.7490	 0.5570
CQ	 0.6420	 0.5420
CR	 0.4790	 0.4400
Ca	 0.6410	 0.5160
Cb	 0.4680	 0.4420
Cd	 0.7570	 0.5370
Cj	 0.7930	 0.5500
Cn	 0.1090	 0.4470
Cp	 0.6910	 0.5300
DD	 0.7410	 0.5470
DI	 0.7130	 0.5250
DL	 0.5230	 0.5070
DO	 0.5440	 0.4470
DP	 0.7720	 0.5190
DR	 0.7680	 0.5400
DU	 0.6030	 0.5080
DZ	 0.4820	 0.5020
F1	 0.4230	 0.4860
F2	 0.6900	 0.5150
F3	 0.5810	 0.4640
F5	 0.2910	 0.3750
F6	 0.4470	 0.3890
F7	 0.6710	 0.5050
F8	 0.5690	 0.5030
F9	 0.5700	 0.5100
FA	 0.1770	 0.4120



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Chain	Atom inclusion	Q-score
FB	 0.5500	 0.5160
FC	 0.4660	 0.4440
FE	 0.6090	 0.5240
FF	 0.3730	 0.4860
FJ	 0.3570	 0.4750
FM	 0.6420	 0.5140
FN	 0.4920	 0.4310
FO	 0.7280	 0.5410
FP	 0.7210	 0.5160
FPA	 1.0000	 0.6700
FQ	 0.4880	 0.4600
FR	 0.4110	 0.4420
FS	 0.3410	 0.4240
FT	 0.4500	 0.4330
FU	 0.3640	 0.4180
FW	 0.6990	 0.5360
FWA	 1.0000	 0.5460
FWB	 1.0000	 0.6970
FX	 0.7690	 0.5160
FY	 0.4200	 0.4330
FZ	 0.0480	 0.4030
Fa	 0.4440	 0.5050
Fb	 0.4770	 0.3940
Fc	 0.4900	 0.3850
FcA	 0.2810	 0.4790
Fd	 0.6820	 0.5140
FdA	 1.0000	 0.6870
UA	 0.1110	 0.2570
UB	 0.0060	 0.2460
UC	 0.6500	 0.4240
UD	 0.7960	 0.4990
UE	 0.0820	 0.2610
UF	 0.4700	 0.4310
UG	 0.4710	 0.4580
UH	 0.2330	 0.4530
UI	 0.5000	 0.4280
UJ	 0.0520	 0.3050
UL	 0.3710	 0.4080
UM	 0.5370	 0.4520
UN	 0.4170	 0.3840
UO	 0.2220	 0.3200
UP	 0.1630	 0.3500

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Chain	Atom inclusion	Q-score
UQ	 0.4810	 0.3800
UU	 0.2430	 0.4200
UY	 0.0010	 0.2780