



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 06:41 AM UTC

PDB ID : 6SG9 / pdb_00006sg9
EMDB ID : EMD-10175
Title : Head 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

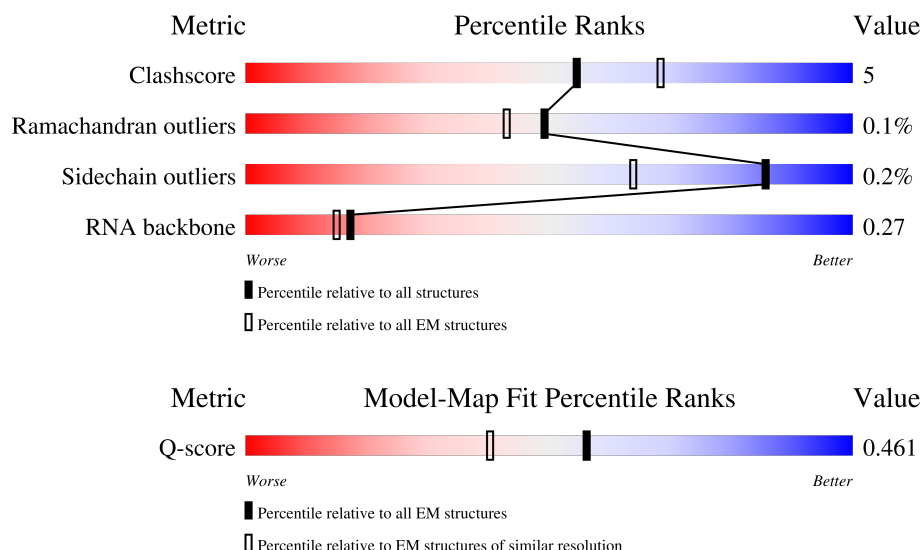
1 Overall quality at a glance

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.



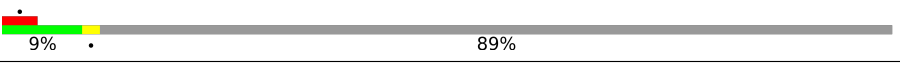
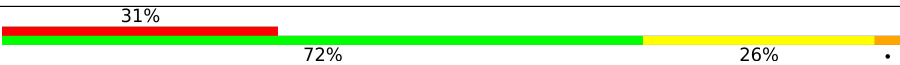
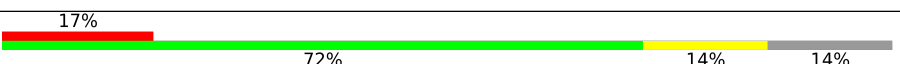
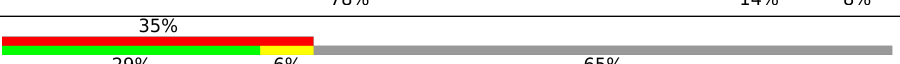
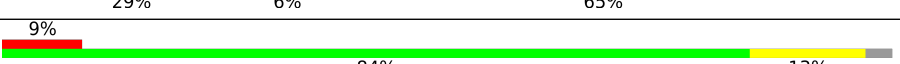
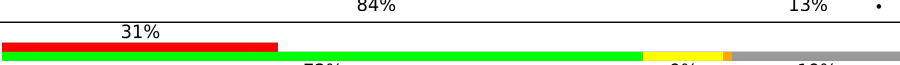
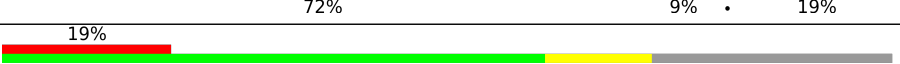
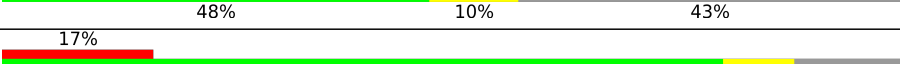
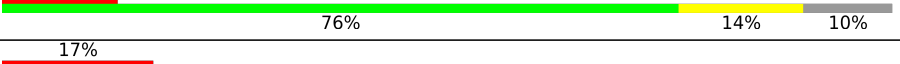
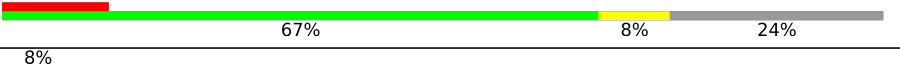
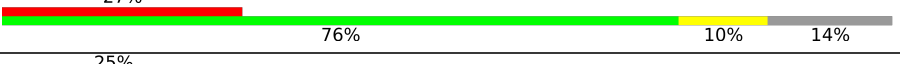
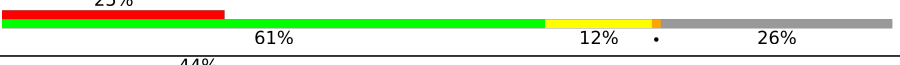
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	
2	CK	326	
3	Cn	250	

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Mol	Chain	Length	Quality of chain
4	FJ	362	
5	FY	188	
6	Fa	171	
7	CA	802	
8	CC	74	
9	CI	443	
10	CJ	817	
11	CN	166	
12	CS	244	
13	Cg	498	
14	Ci	181	
15	Ck	874	
16	DB	1181	
17	DC	1165	
18	DE	747	
19	DF	666	
20	DG	631	
21	DH	581	
22	DJ	396	
23	DK	324	
24	DT	247	
25	DV	183	
26	DW	179	
27	DX	169	
28	DY	163	

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Mol	Chain	Length	Quality of chain
29	F1	1041	
30	F4	811	
31	FD	579	
32	FF	474	
33	FG	463	
34	FH	457	
35	FI	445	
36	FK	372	
37	FL	353	
38	FV	264	
39	Fe	123	
40	Ua	70	
41	Ub	42	
42	Uc	12	
43	Ud	59	
44	Ue	29	
45	Uf	9	
46	Ug	167	
47	Uh	255	
48	Ui	32	
49	Uj	19	
50	Uk	27	
51	Ul	14	
52	Um	11	
53	Ux	108	

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 104694 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	23	Total	C	N	O	S	0	0
			200	132	35	31	2		

- Molecule 2 is a protein called uS11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	CK	40	Total	C	N	O	S	0	0
			337	209	65	62	1		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 3 is a protein called mS38.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	Cn	18	Total	C	N	O	0	0
			154	103	28	23		

- Molecule 4 is a protein called mt-SAF18.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	FJ	41	Total	C	N	O	S	0	0
			338	208	61	67	2		

- Molecule 5 is a protein called mt-SAF28.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	FY	92	Total	C	N	O	S	0	0
			723	463	123	131	6		

- Molecule 6 is a protein called mt-SAF30.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Fa	39	Total	C	N	O	S	0	0
			297	192	55	49	1		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 7 is a RNA chain called 9S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	CA	146	Total	C	N	O	P	0	0
			2501	1098	308	949	146		

- Molecule 8 is a protein called uS3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	CC	74	Total	C	N	O	S	0	0
			646	451	96	98	1		

- Molecule 9 is a protein called uS9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	CI	423	Total	C	N	O	S	0	0
			3357	2108	601	631	17		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CI	370	ALA	VAL	conflict	UNP Q57W62

- Molecule 10 is a protein called uS10m.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	CJ	701	Total	C	N	O	S	0	0
			5709	3605	1017	1064	23		

- Molecule 11 is a protein called uS14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	CN	153	Total	C	N	O	S	0	0
			1285	820	242	216	7		

- Molecule 12 is a protein called uS19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	CS	85	Total	C	N	O	S	0	0
			708	463	121	121	3		

- Molecule 13 is a protein called mS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Cg	484	Total	C	N	O	S	0	0
			3922	2511	688	703	20		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Cg	181	VAL	ALA	conflict	UNP Q585C2
Cg	498	ARG	MET	conflict	UNP Q585C2

- Molecule 14 is a protein called mS33.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Ci	147	Total	C	N	O	S	0	0
			1222	770	226	218	8		

- Molecule 15 is a protein called mS35.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Ck	638	Total	C	N	O	S	0	0
			5123	3220	927	953	23		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ck	107	SER	LEU	conflict	UNP Q387C7
Ck	144	PHE	LEU	conflict	UNP Q387C7
Ck	253	TYR	PHE	conflict	UNP Q387C7
Ck	339	GLU	VAL	conflict	UNP Q387C7
Ck	871	GLY	GLU	conflict	UNP Q387C7

- Molecule 16 is a protein called mS49.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	DB	679	Total	C	N	O	S	0	0
			5688	3558	1062	1047	21		

- Molecule 17 is a protein called mS50.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	DC	1028	Total	C	N	O	S	0	0
			8223	5194	1453	1546	30		

- Molecule 18 is a protein called mS52.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	DE	590	Total	C	N	O	S	0	0
			4639	2957	832	834	16		

- Molecule 19 is a protein called mS53.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	DF	491	Total	C	N	O	S	0	0
			3967	2496	745	703	23		

- Molecule 20 is a protein called mS54.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	DG	566	Total	C	N	O	S	0	0
			4575	2875	835	834	31		

- Molecule 21 is a protein called mS55 (KRIPP8).

Mol	Chain	Residues	Atoms					AltConf	Trace
21	DH	472	Total	C	N	O	S	0	0
			3849	2417	720	693	19		

- Molecule 22 is a protein called mS57.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	DJ	308	Total	C	N	O	S	0	0
			2521	1612	446	450	13		

- Molecule 23 is a protein called mS58.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	DK	245	Total	C	N	O	S	0	0
			1929	1213	349	362	5		

- Molecule 24 is a protein called mS67.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	DT	221	Total	C	N	O	S	0	0
			1912	1231	334	337	10		

- Molecule 25 is a protein called mS69.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	DV	157	Total	C	N	O	S	0	0
			1323	840	248	231	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DV	163	ALA	THR	conflict	UNP Q57UZ6

- Molecule 26 is a protein called mS70.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	DW	133	Total	C	N	O	S	0	0
			1140	730	216	190	4		

- Molecule 27 is a protein called mS71.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	DX	115	Total	C	N	O	S	0	0
			967	612	182	166	7		

- Molecule 28 is a protein called mS72.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	DY	154	Total	C	N	O	S	0	0
			1295	829	247	214	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DY	34	HIS	ASP	conflict	UNP Q57YD4

- Molecule 29 is a protein called mt-SAF1 (RSM22).

Mol	Chain	Residues	Atoms					AltConf	Trace
29	F1	833	Total	C	N	O	S	0	0
			6729	4212	1265	1213	39		

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 30 is a protein called mt-SAF4.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	F4	541	Total	C	N	O	S	0	0
			4382	2783	775	802	22		

- Molecule 31 is a protein called mt-SAF12 (KRIPP18).

Mol	Chain	Residues	Atoms					AltConf	Trace
31	FD	394	Total	C	N	O	S	0	0
			3135	2004	546	566	19		

- Molecule 32 is a protein called mt-SAF14.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	FF	408	Total	C	N	O	S	0	0
			3265	2052	586	603	24		

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 33 is a protein called mt-SAF15.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	FG	169	Total	C	N	O	S	0	0
			1359	852	260	240	7		

- Molecule 34 is a protein called mt-SAF16.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	FH	317	Total	C	N	O	S	0	0
			2486	1555	440	471	20		

- Molecule 35 is a protein called mt-SAF17.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	FI	348	Total	C	N	O	S	0	0
			2786	1726	510	537	13		

- Molecule 36 is a protein called mt-SAF19.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	FK	208	Total	C	N	O	S	0	0
			1699	1084	284	325	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
FK	38	HIS	ARG	conflict	UNP Q57XS8

- Molecule 37 is a protein called mt-SAF20.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	FL	320	Total	C	N	O	S	0	0
			2555	1609	470	459	17		

- Molecule 38 is a protein called mt-SAF25.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	FV	210	Total	C	N	O	S	0	0
			1636	1039	283	303	11		

- Molecule 39 is a protein called mt-SAF34.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Fe	122	Total	C	N	O	S	0	0
			1033	642	200	184	7		

- Molecule 40 is a protein called UNK-a.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	Ua	47	Total	C	N	O	0	0
			282	188	47	47		

- Molecule 41 is a protein called UNK-b.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	Ub	42	Total	C	N	O	0	0
			252	168	42	42		

- Molecule 42 is a protein called UNK-c.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	Uc	12	Total	C	N	O	0	0
			72	48	12	12		

- Molecule 43 is a protein called UNK-d.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	Ud	59	Total	C	N	O	0	0
			354	236	59	59		

- Molecule 44 is a protein called UNK-e.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	Ue	29	Total	C	N	O	0	0
			174	116	29	29		

- Molecule 45 is a protein called UNK-f.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	Uf	9	Total	C	N	O	0	0
			54	36	9	9		

- Molecule 46 is a protein called UNK-g.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	Ug	167	Total	C	N	O	0	0
			1002	668	167	167		

- Molecule 47 is a protein called UNK-h.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	Uh	255	Total	C	N	O	0	0
			1530	1020	255	255		

- Molecule 48 is a protein called UNK-i.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	Ui	32	Total	C	N	O	0	0
			192	128	32	32		

- Molecule 49 is a protein called UNK-j.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	Uj	19	Total	C	N	O	0	0
			114	76	19	19		

- Molecule 50 is a protein called UNK-k.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	Uk	27	Total	C	N	O	0	0
			162	108	27	27		

- Molecule 51 is a protein called UNK-l.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	Ul	14	Total	C	N	O	0	0
			84	56	14	14		

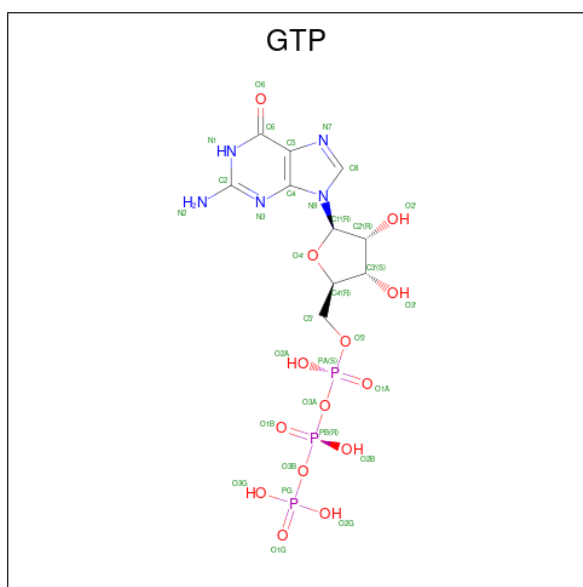
- Molecule 52 is a protein called UNK-m.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	Um	11	Total	C	N	O	0	0
			66	44	11	11		

- Molecule 53 is a protein called UNK-x.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	Ux	108	Total	C	N	O	0	0
			648	432	108	108		

- Molecule 54 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					AltConf
54	CgA	1	Total	C	N	O	P	0
			32	10	5	14	3	

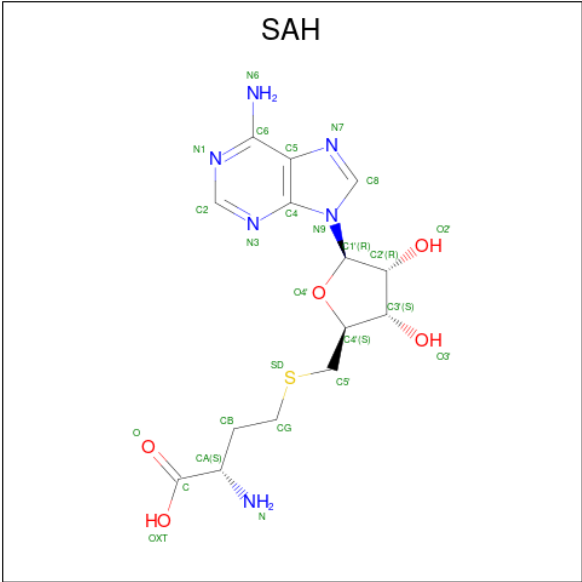
- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
55	CgB	1	Total	Mg	0
			1	1	

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
56	F1A	1	Total	Zn	0
			1	1	
56	FGA	1	Total	Zn	0
			1	1	
56	FLA	1	Total	Zn	0
			1	1	
56	FLB	1	Total	Zn	0
			1	1	
56	FeA	1	Total	Zn	0
			1	1	

- Molecule 57 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: C₁₄H₂₀N₆O₅S).

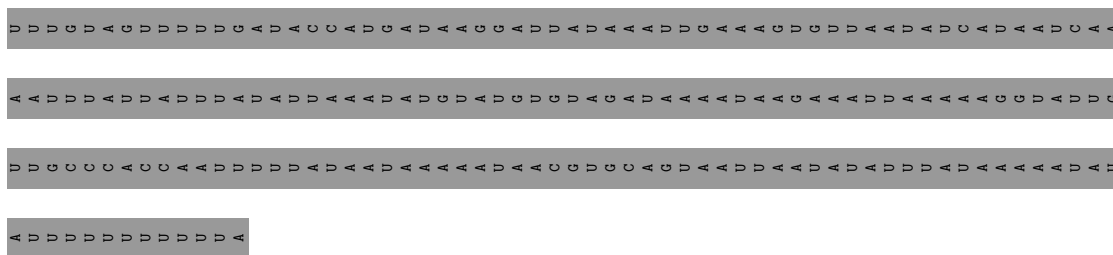


Mol	Chain	Residues	Atoms					AltConf
57	F1B	1	Total	C	N	O	S	0
			26	14	6	5	1	
57	FFA	1	Total	C	N	O	S	0
			26	14	6	5	1	

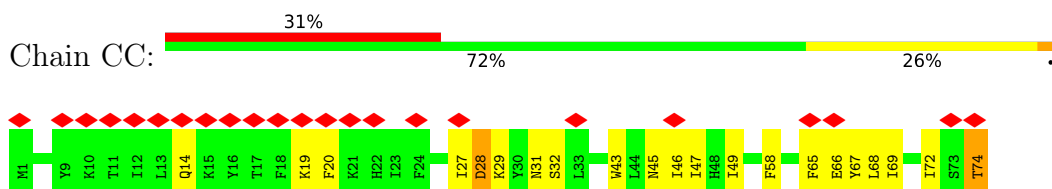
- Molecule 58 is water.

Mol	Chain	Residues	Atoms		AltConf
58	CgC	3	Total	O	0
			3	3	

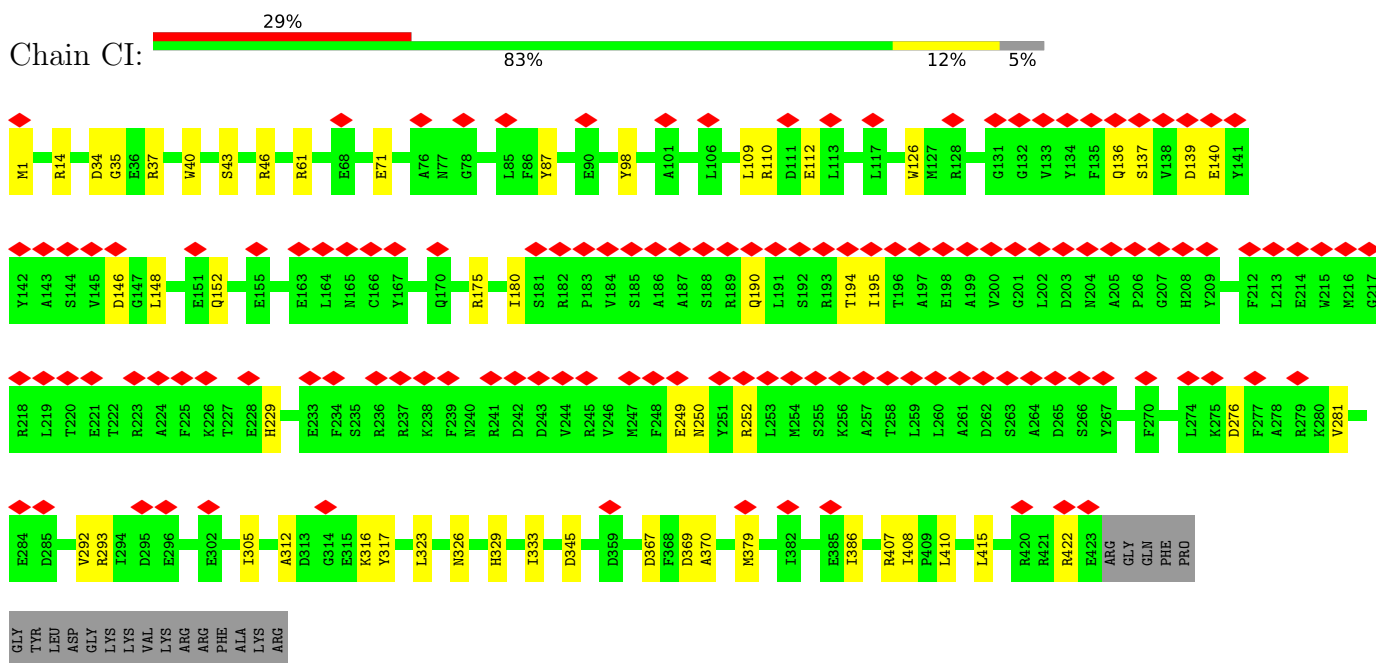




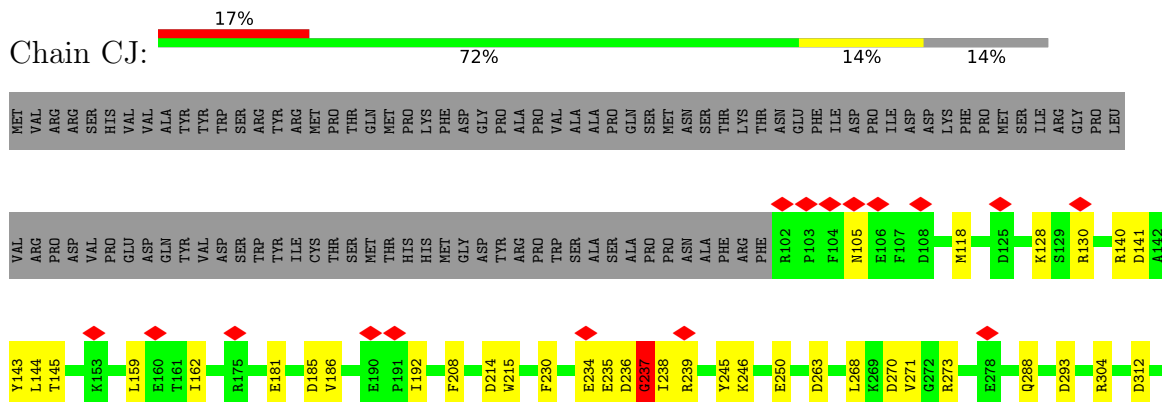
- Molecule 8: uS3m

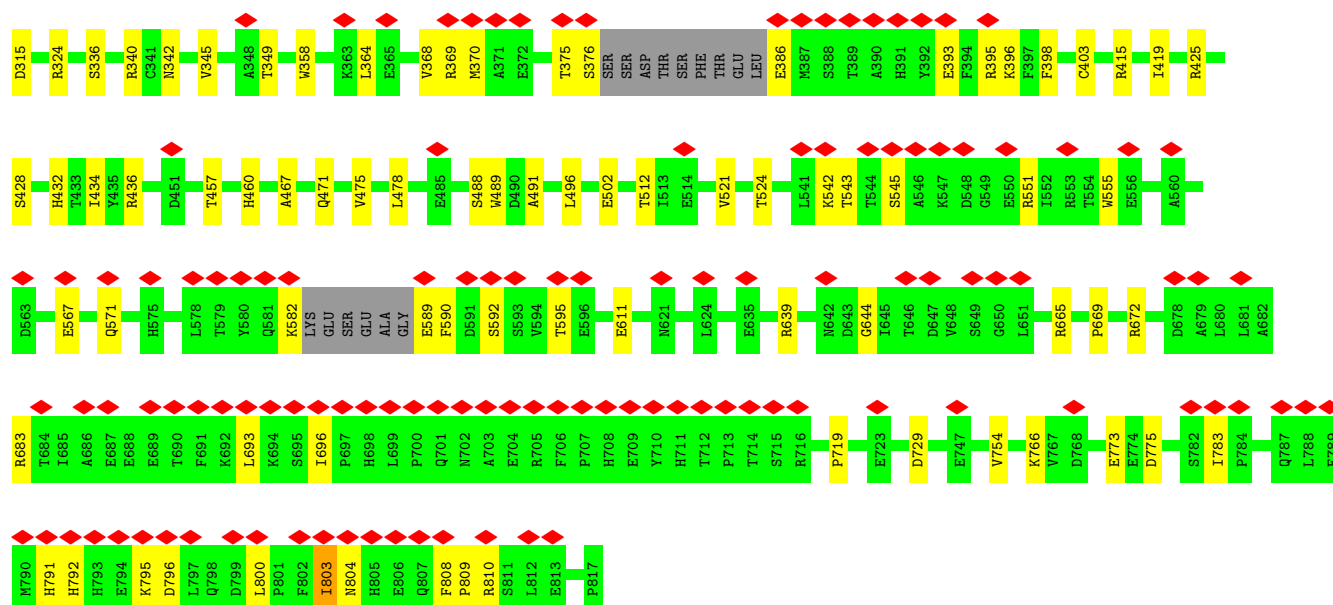


- Molecule 9: uS9m

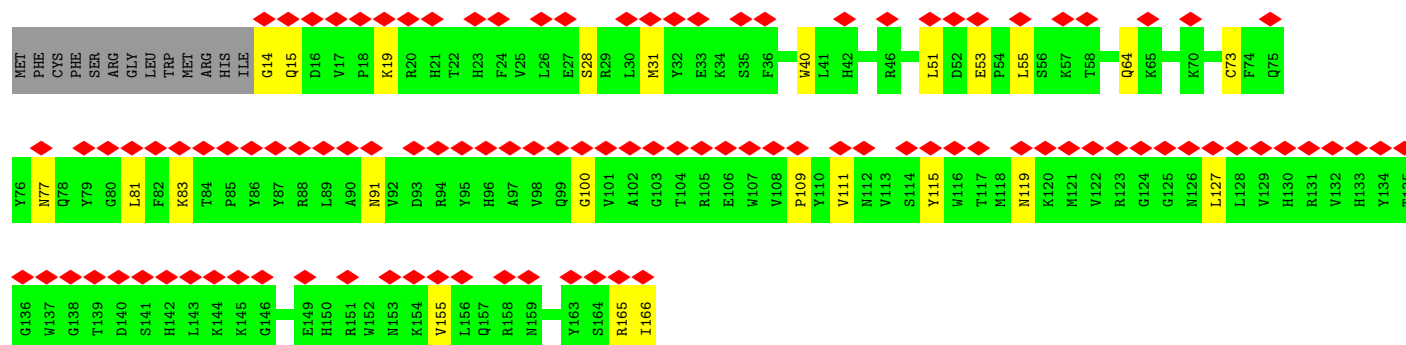
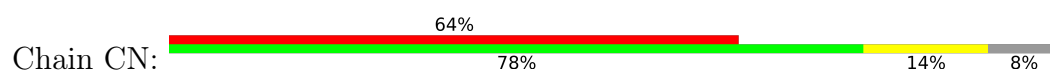


- Molecule 10: uS10m

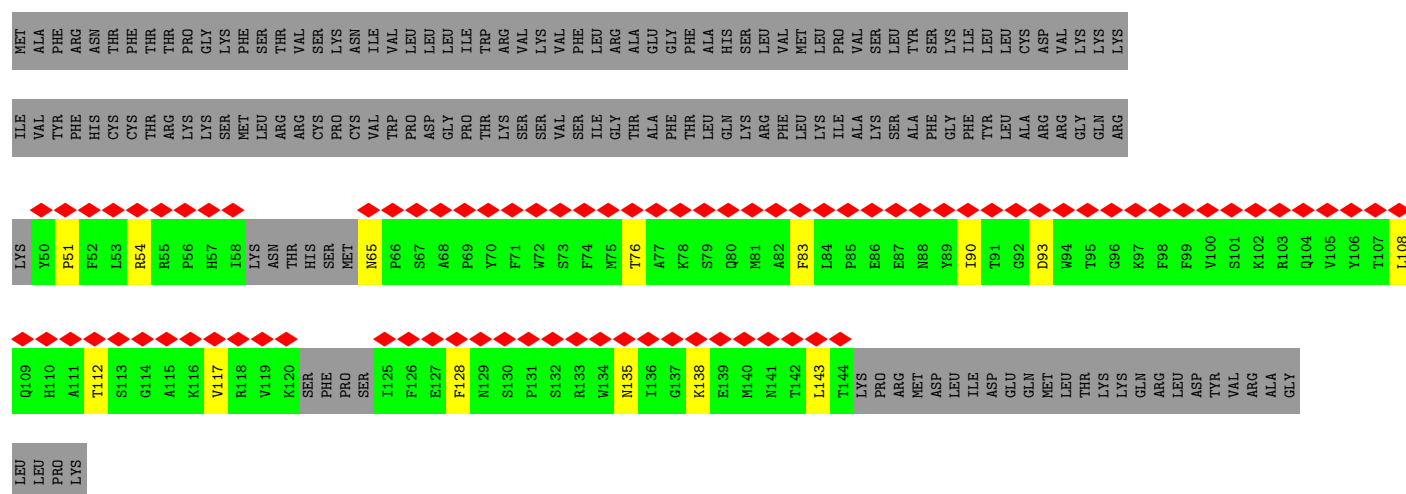




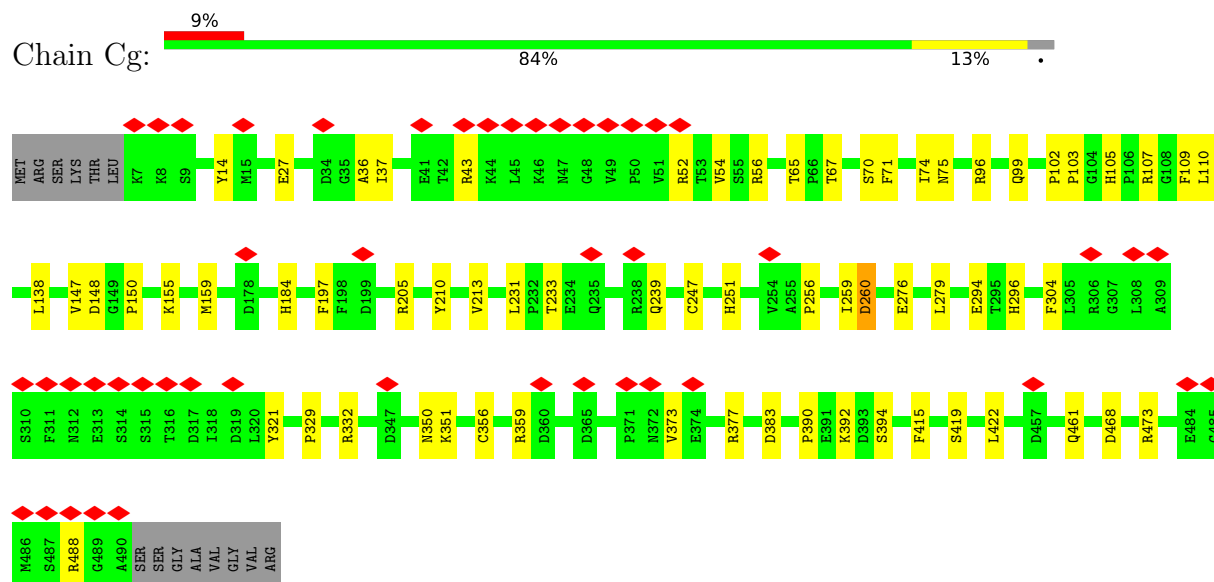
• Molecule 11: uS14m



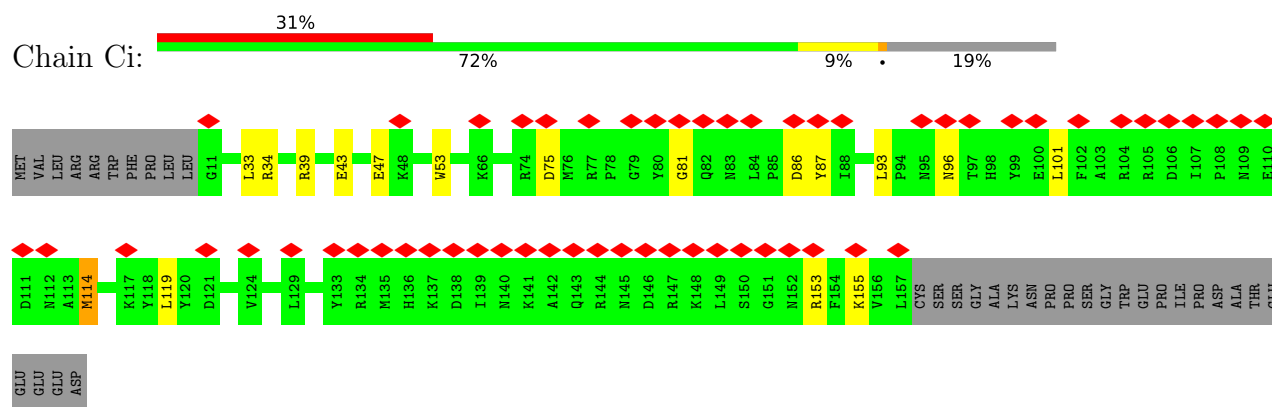
• Molecule 12: uS19m



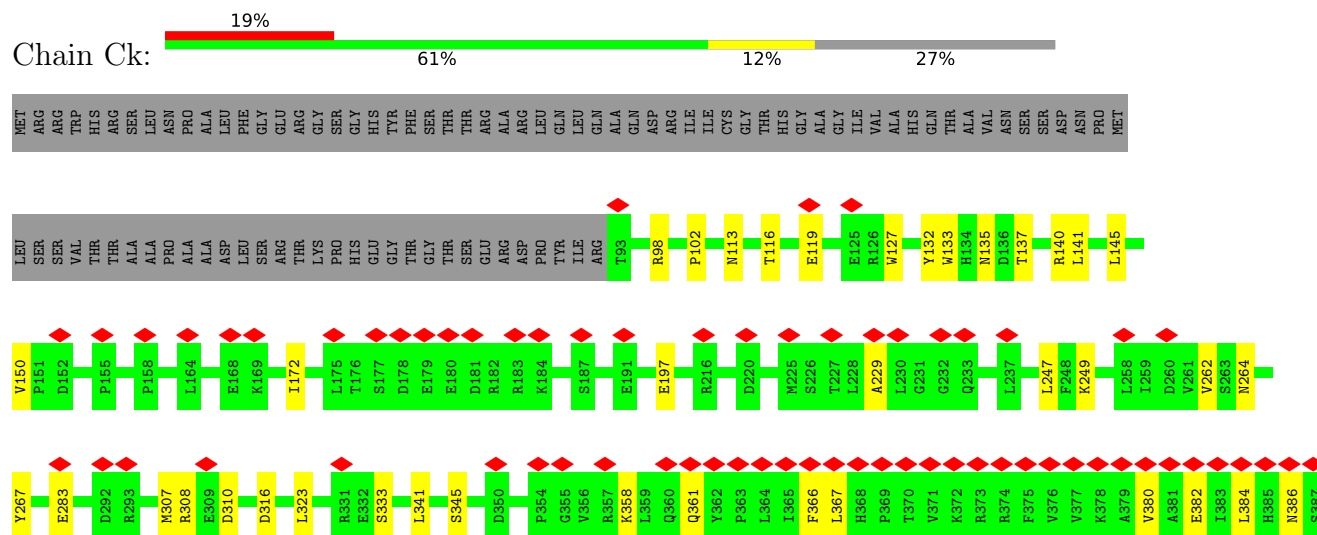
- Molecule 13: mS29

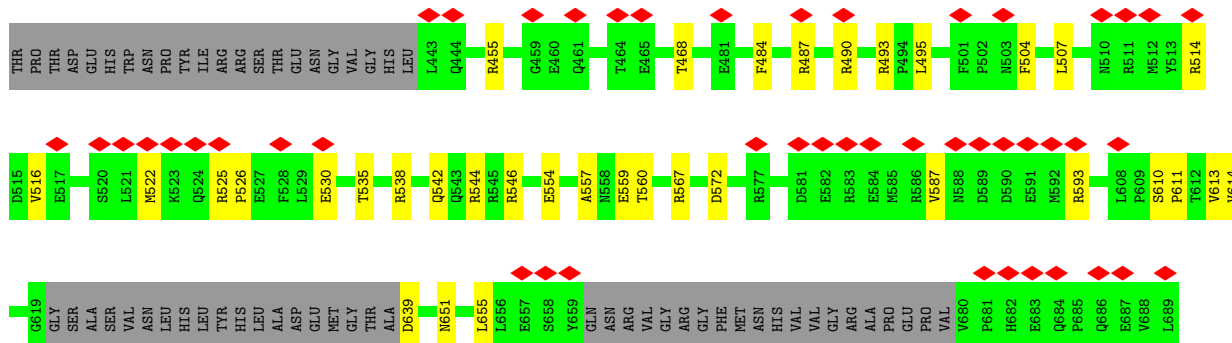


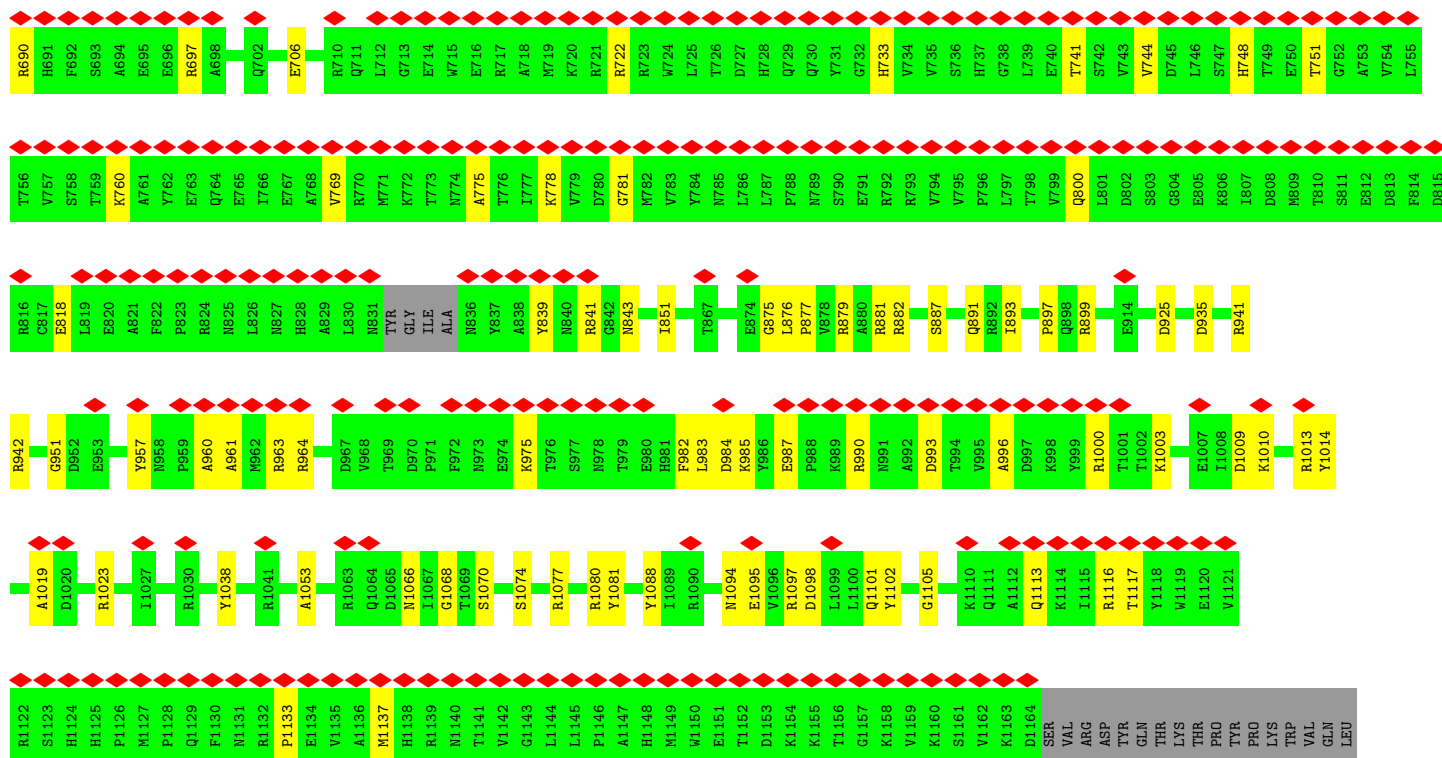
- Molecule 14: mS33



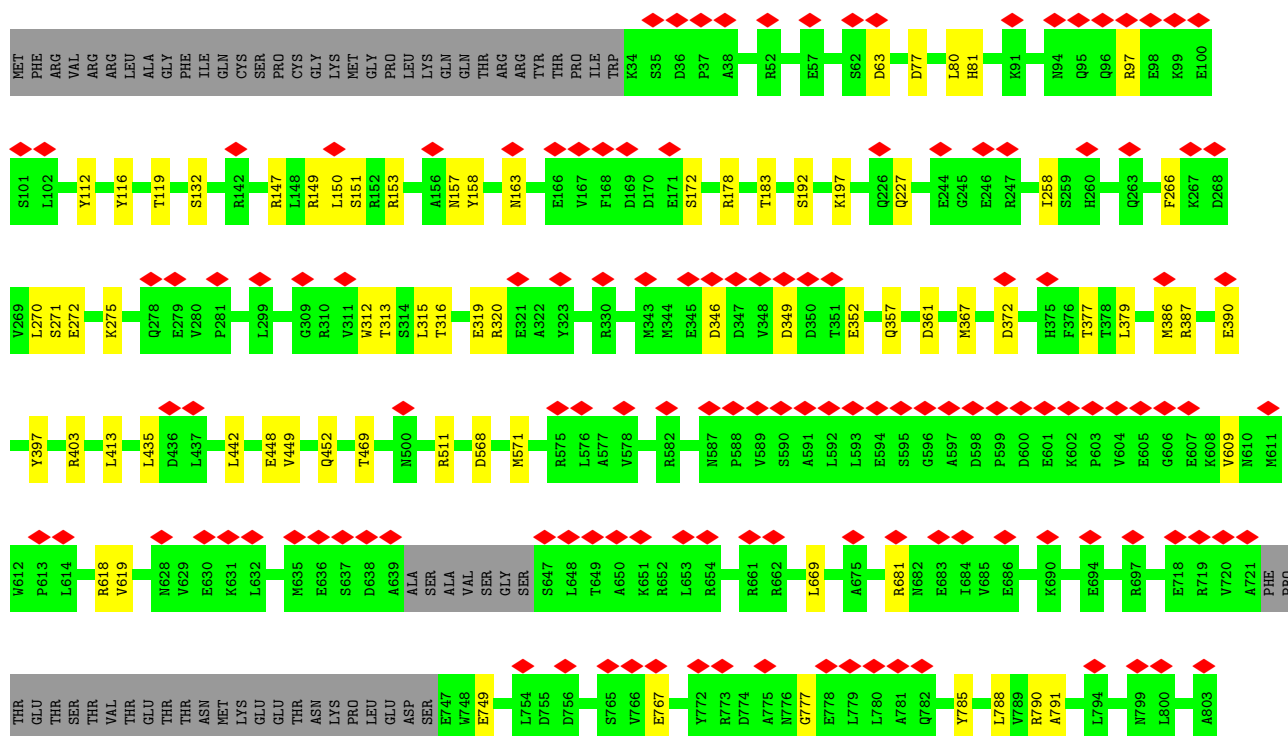
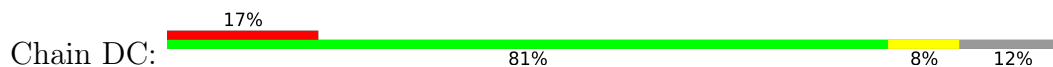
- Molecule 15: mS35



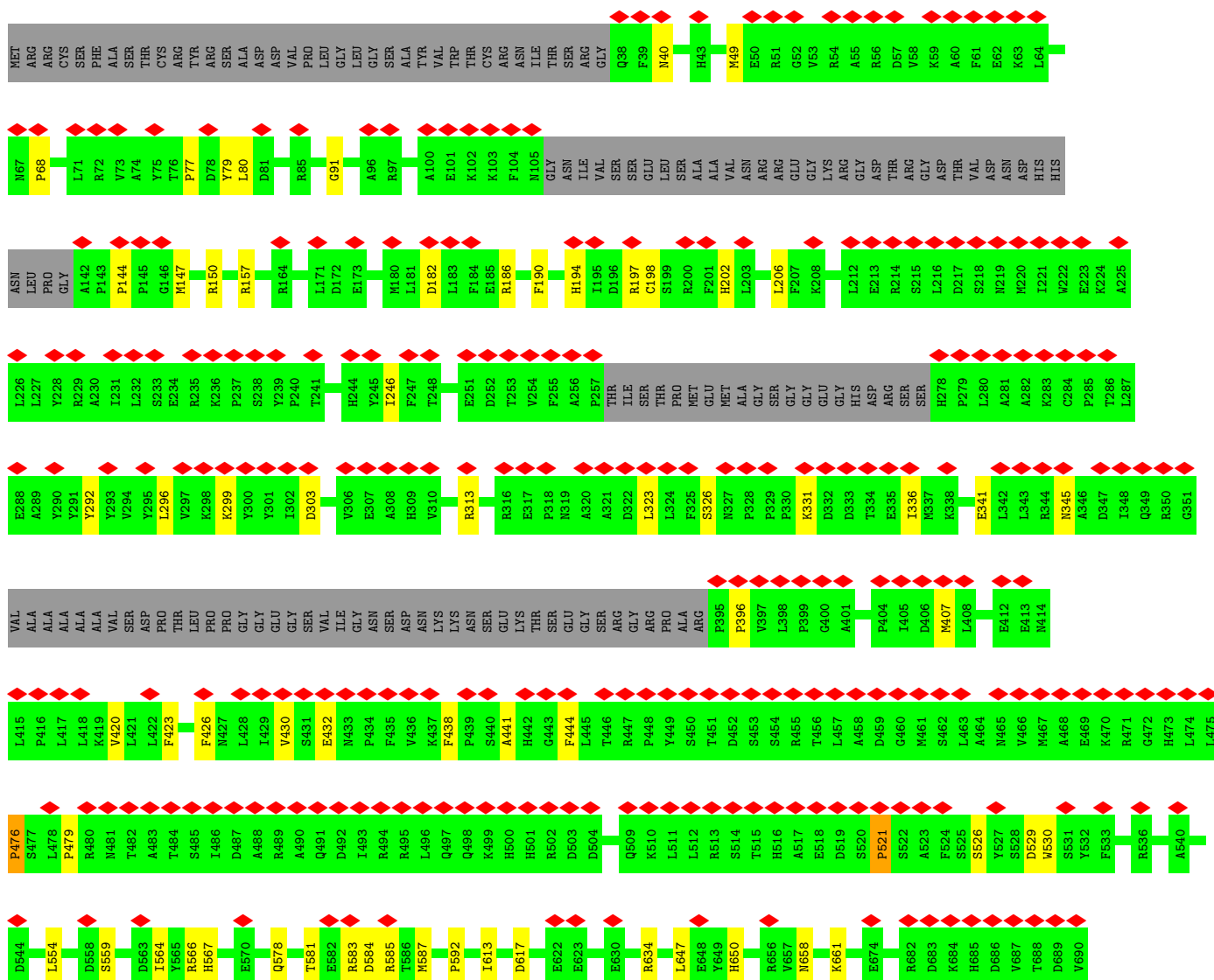
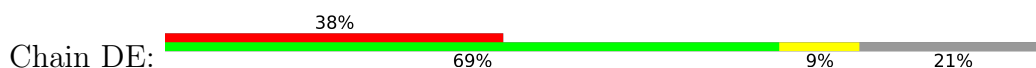




• Molecule 17: mS50

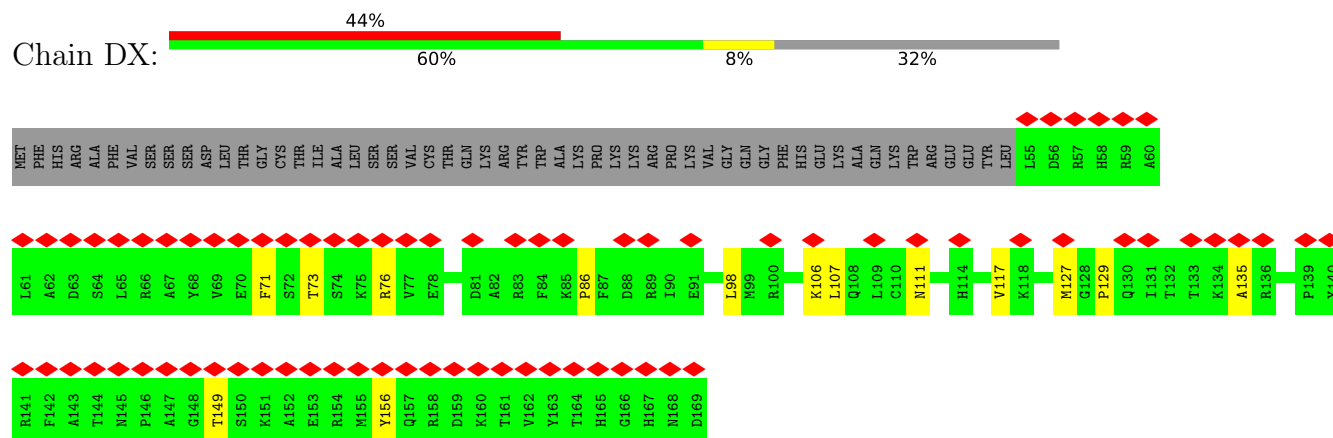


- Molecule 18: mS52



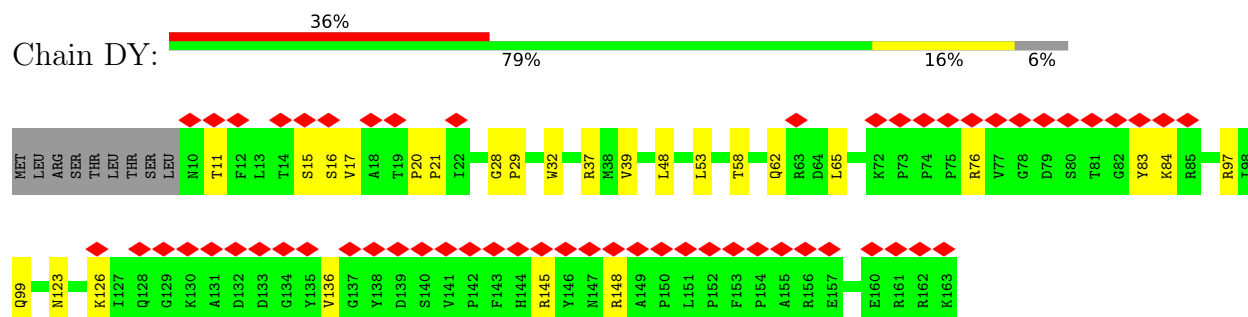
- Molecule 27: mS71

Chain DX:



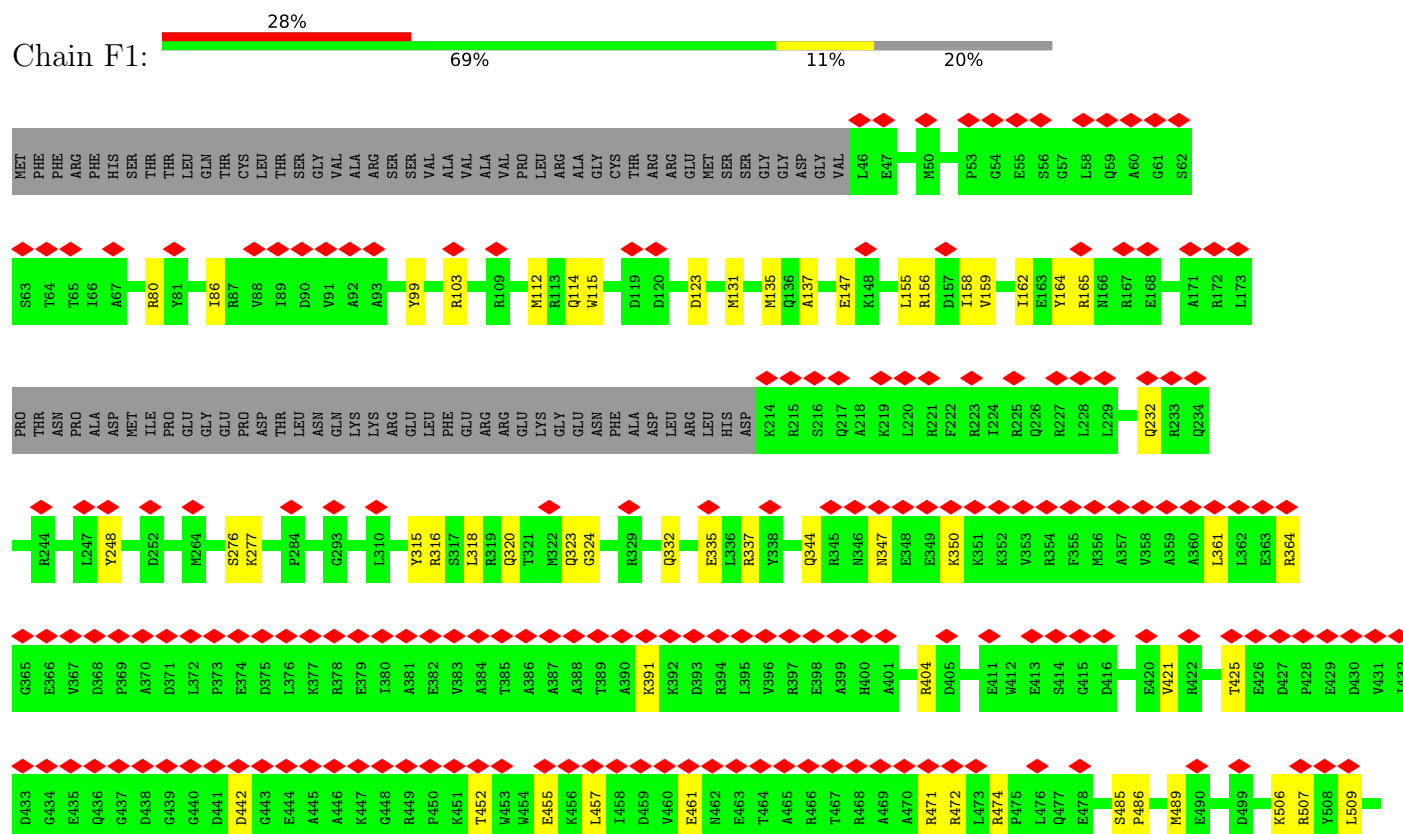
- Molecule 28: mS72

Chain DY:

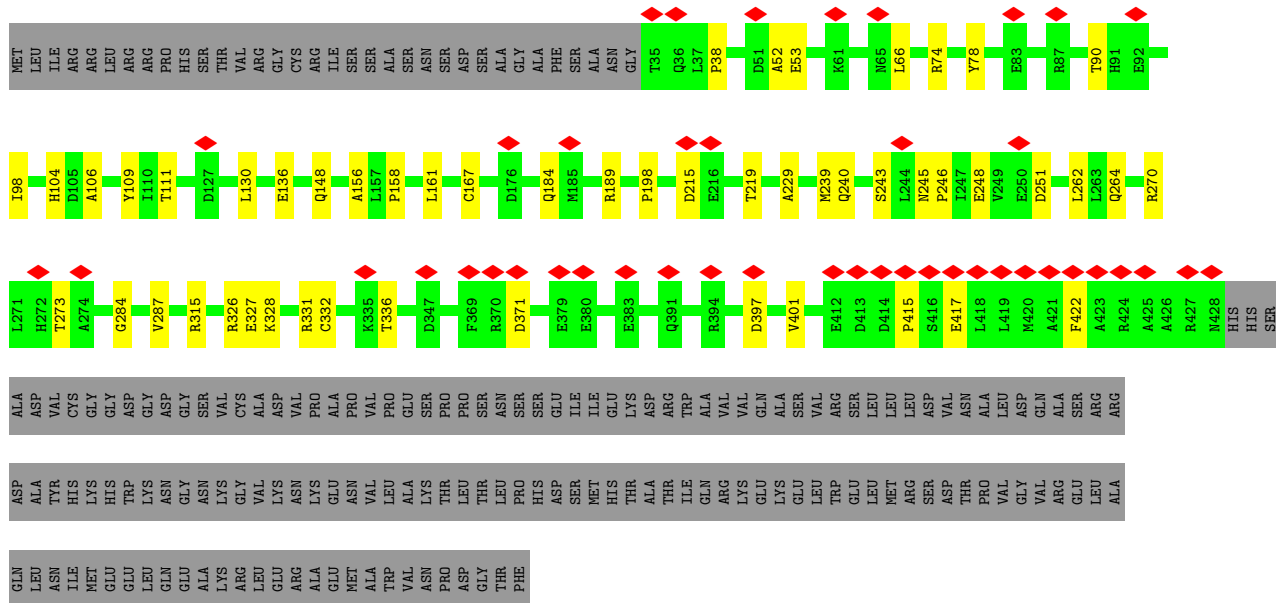


- Molecule 29: mt-SAF1 (RSM22)

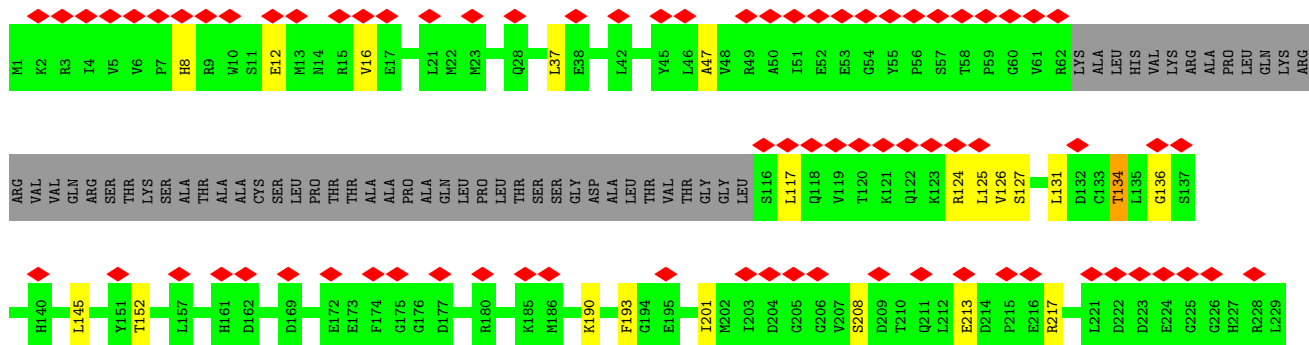
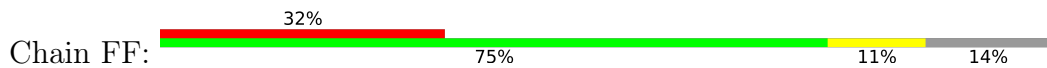
Chain F1:



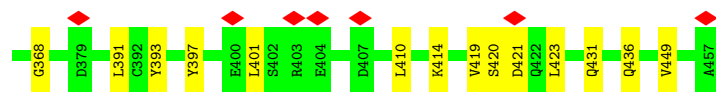
- Molecule 31: mt-SAF12 (KRIPP18)



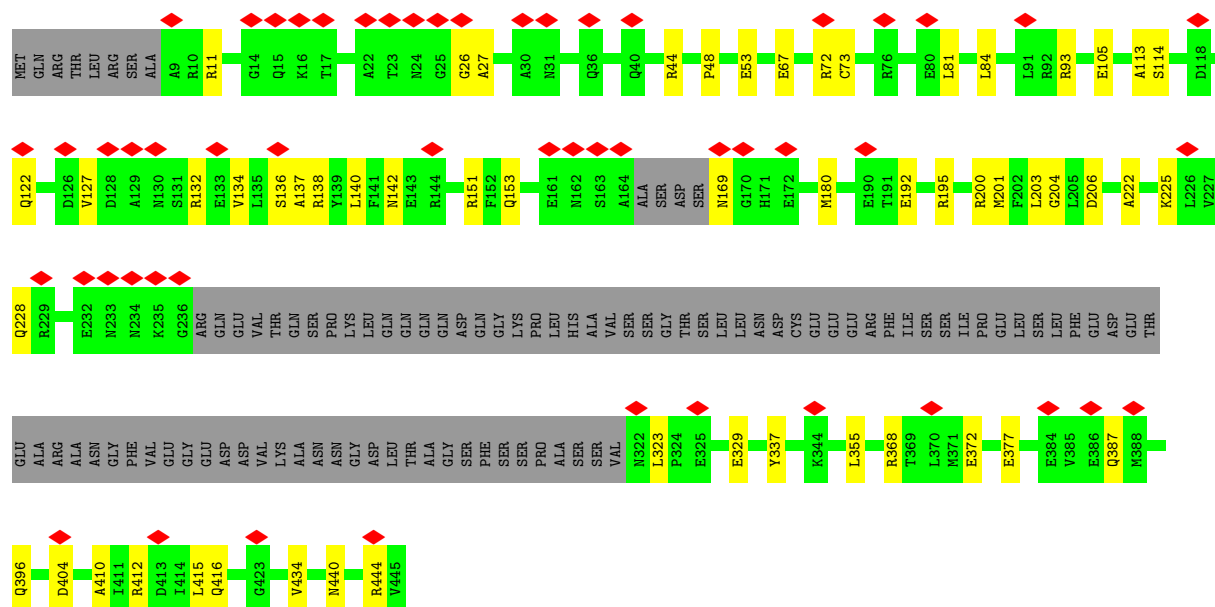
- Molecule 32: mt-SAF14



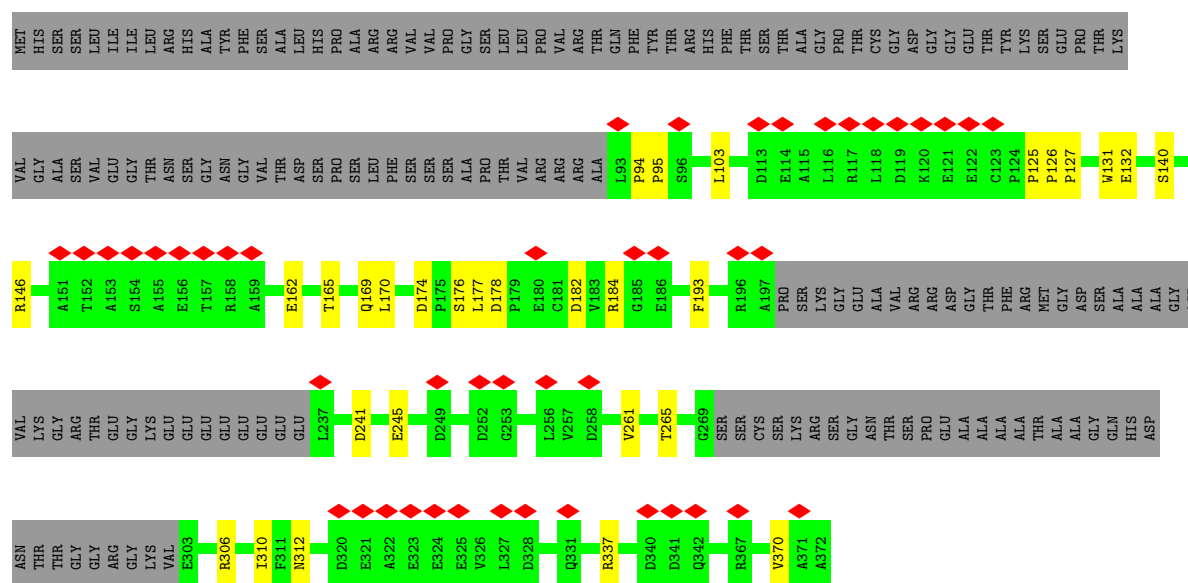




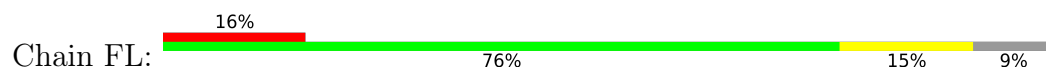
• Molecule 35: mt-SAF17

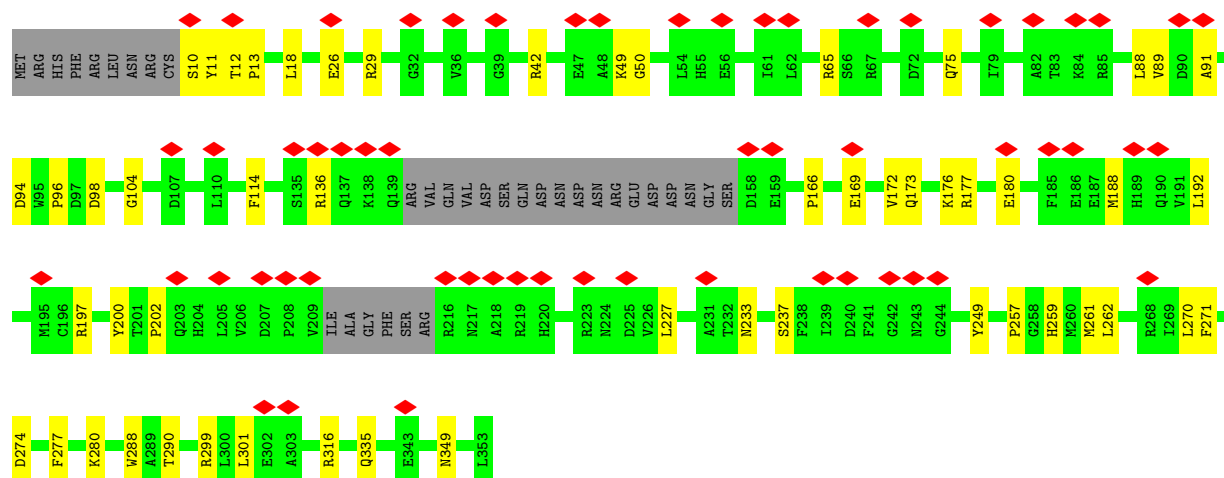


• Molecule 36: mt-SAF19

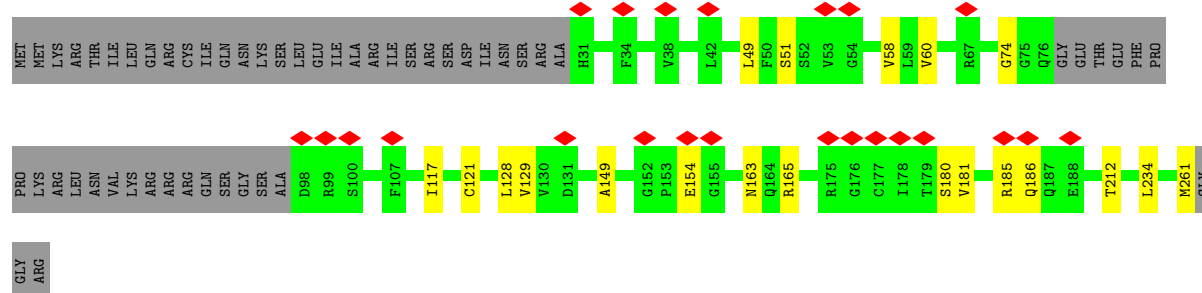
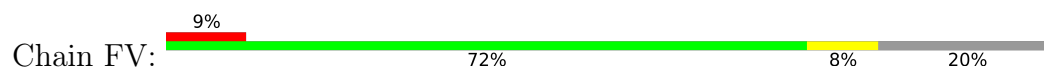


• Molecule 37: mt-SAF20

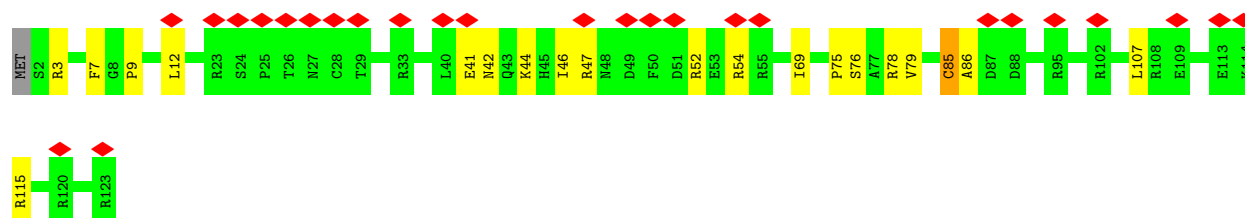
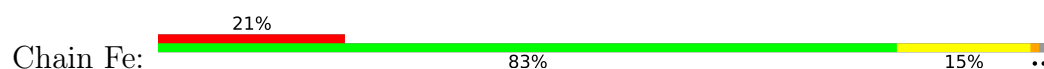




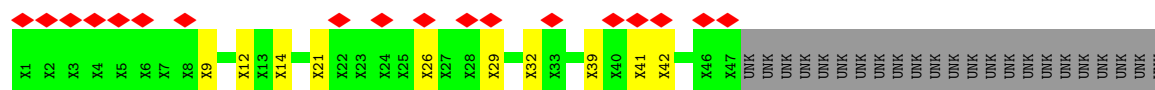
- Molecule 38: mt-SAF25



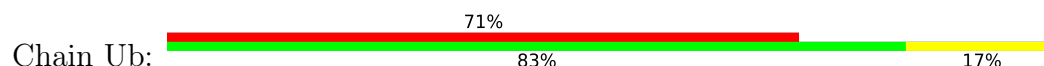
- Molecule 39: mt-SAF34



- Molecule 40: UNK-a

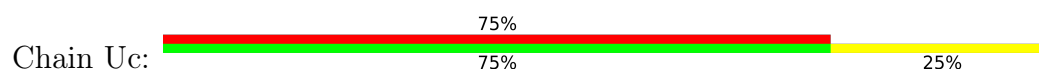


- Molecule 41: UNK-b

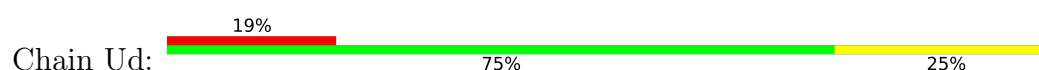




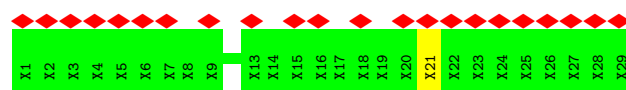
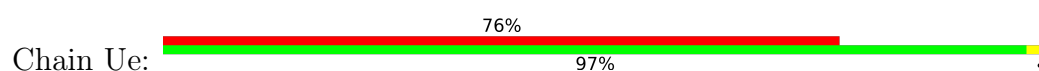
• Molecule 42: UNK-c



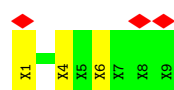
• Molecule 43: UNK-d



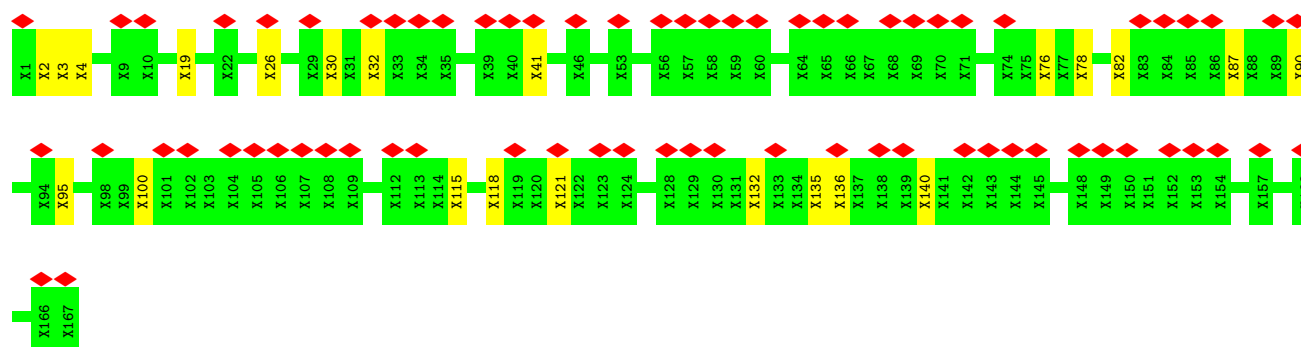
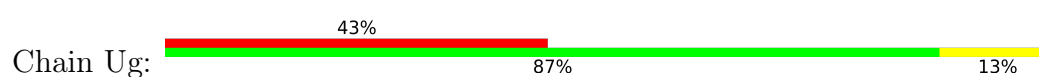
• Molecule 44: UNK-e



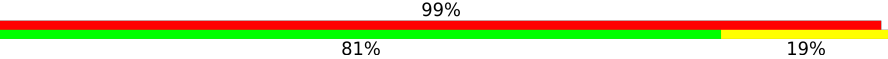
• Molecule 45: UNK-f

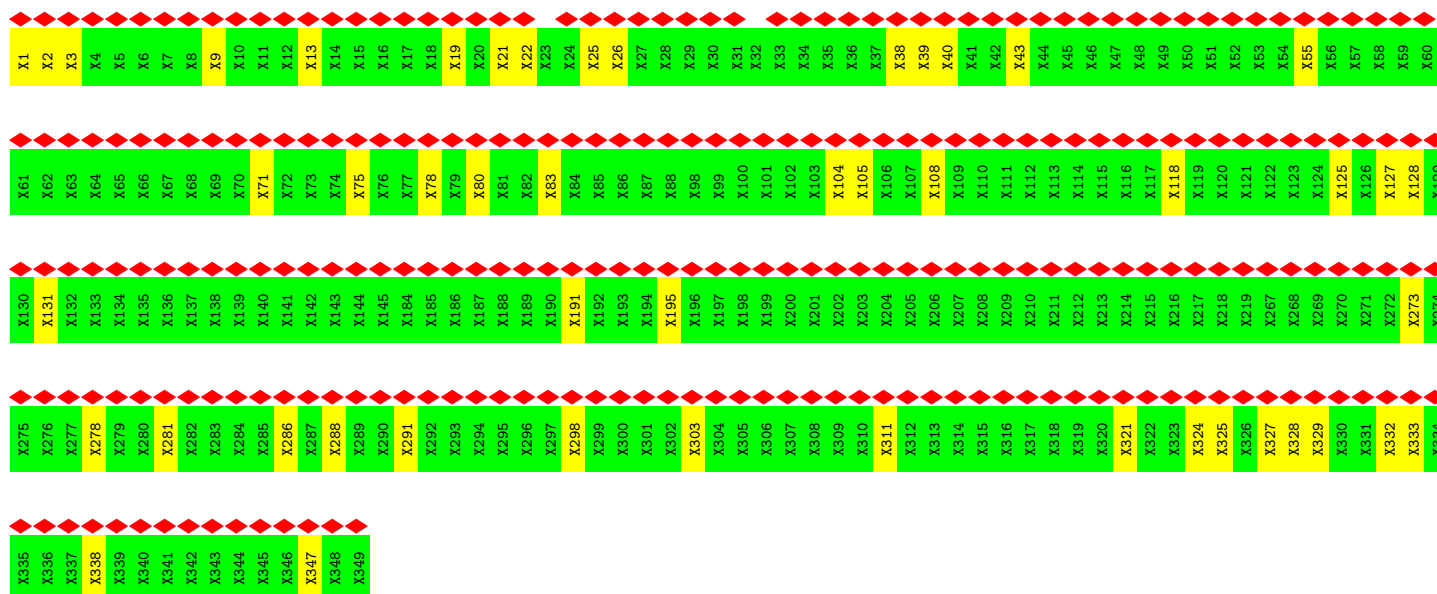


• Molecule 46: UNK-g



• Molecule 47: UNK-h

Chain Uh: 



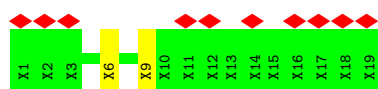
• Molecule 48: UNK-i

Chain Ui: 



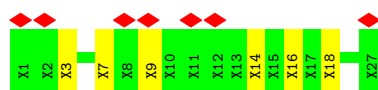
• Molecule 49: UNK-j

Chain Uj: 



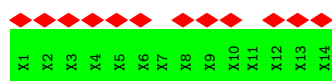
• Molecule 50: UNK-k

Chain Uk: 

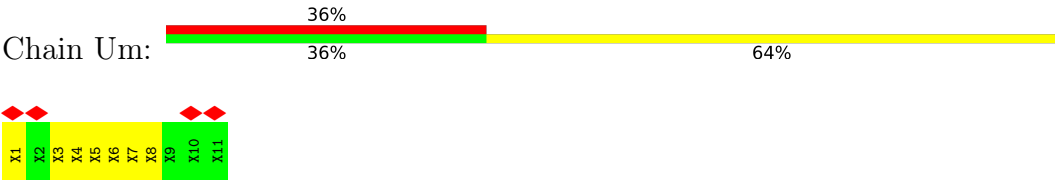


• Molecule 51: UNK-l

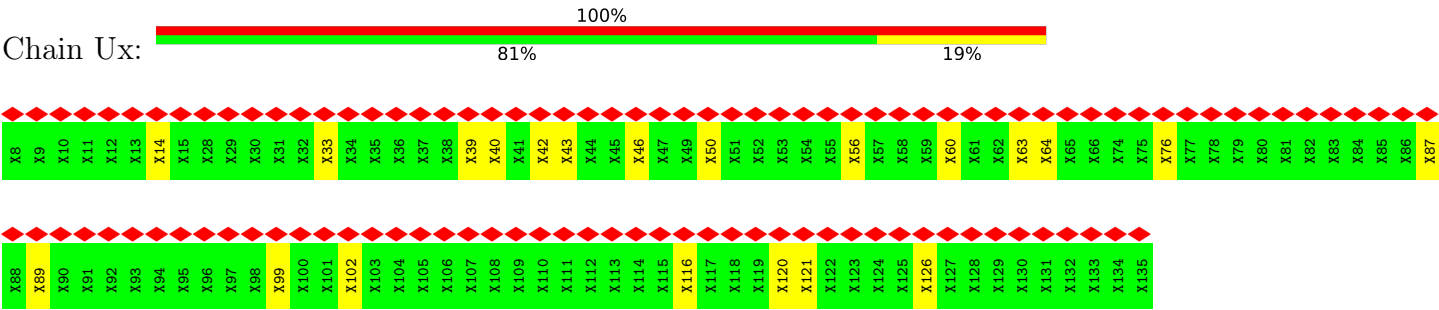
Chain Ul: 



● Molecule 52: UNK-m



● Molecule 53: UNK-x



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	0.420	Depositor
Minimum map value	-0.186	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.0793	Depositor
Map size (Å)	444.8, 444.8, 444.8	wwPDB
Map dimensions	320, 320, 320	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: GTP, ZN, MG, SAH

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	0.14	0/206	0.37	0/278
2	CK	0.20	0/343	0.43	0/461
3	Cn	0.19	0/161	0.50	0/218
4	FJ	0.18	0/340	0.43	0/454
5	FY	0.20	0/736	0.49	0/987
6	Fa	0.16	0/307	0.39	0/417
7	CA	0.14	0/2774	0.34	0/4302
8	CC	0.40	0/666	0.55	0/900
9	CI	0.18	0/3424	0.43	0/4626
10	CJ	0.18	0/5865	0.44	0/7974
11	CN	0.17	0/1323	0.42	0/1790
12	CS	0.16	0/731	0.40	0/987
13	Cg	0.18	0/4043	0.41	0/5489
14	Ci	0.18	0/1256	0.43	0/1695
15	Ck	0.19	0/5215	0.47	0/7050
16	DB	0.17	0/5830	0.44	0/7889
17	DC	0.16	0/8409	0.40	0/11399
18	DE	0.15	0/4756	0.42	3/6462 (0.0%)
19	DF	0.18	0/4056	0.45	2/5493 (0.0%)
20	DG	0.17	0/4674	0.43	0/6333
21	DH	0.20	0/3935	0.47	0/5321
22	DJ	0.16	0/2591	0.40	0/3508
23	DK	0.17	0/1965	0.41	0/2652
24	DT	0.19	0/1982	0.42	0/2686
25	DV	0.17	0/1358	0.46	0/1836
26	DW	0.18	0/1182	0.46	0/1613
27	DX	0.18	0/993	0.45	0/1336
28	DY	0.16	0/1337	0.40	0/1814
29	F1	0.19	0/6865	0.47	2/9259 (0.0%)
30	F4	0.17	0/4483	0.46	0/6061
31	FD	0.20	0/3216	0.46	1/4380 (0.0%)
32	FF	0.15	0/3335	0.44	0/4498

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	FG	0.17	0/1386	0.43	0/1869
34	FH	0.19	0/2537	0.42	0/3442
35	FI	0.17	0/2834	0.43	0/3821
36	FK	0.15	0/1748	0.35	0/2378
37	FL	0.20	0/2613	0.45	0/3538
38	FV	0.16	0/1680	0.41	0/2281
39	Fe	0.19	0/1057	0.51	0/1421
All	All	0.18	0/102212	0.43	8/138918 (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
10	CJ	0	1
15	Ck	0	1
21	DH	0	1
26	DW	0	1
32	FF	0	1
39	Fe	0	1
All	All	0	6

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	DE	479	PRO	N-CA-CB	7.08	110.68	103.25
18	DE	476	PRO	N-CA-CB	6.67	110.26	103.25
18	DE	521	PRO	N-CA-CB	6.39	109.96	103.25
29	F1	158	ILE	CA-C-N	6.32	124.22	120.24
29	F1	158	ILE	C-N-CA	6.32	124.22	120.24
31	FD	243	SER	N-CA-C	-5.39	100.64	108.07
19	DF	183	SER	CA-C-N	5.16	127.60	120.49
19	DF	183	SER	C-N-CA	5.16	127.60	120.49

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	CJ	237	GLY	Peptide

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Mol	Chain	Res	Type	Group
15	Ck	229	ALA	Peptide
21	DH	484	ASP	Peptide
26	DW	55	TRP	Peptide
32	FF	279	LYS	Peptide
39	Fe	85	CYS	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	200	0	200	2	0
2	CK	337	0	328	3	0
3	Cn	154	0	144	1	0
4	FJ	338	0	344	7	0
5	FY	723	0	738	4	0
6	Fa	297	0	299	5	0
7	CA	2501	0	1249	22	0
8	CC	646	0	682	35	0
9	CI	3357	0	3310	39	0
10	CJ	5709	0	5508	76	0
11	CN	1285	0	1264	16	0
12	CS	708	0	688	11	0
13	Cg	3922	0	3811	49	0
14	Ci	1222	0	1192	16	0
15	Ck	5123	0	5154	76	0
16	DB	5688	0	5497	82	0
17	DC	8223	0	8043	57	0
18	DE	4639	0	4417	47	0
19	DF	3967	0	3957	46	0
20	DG	4575	0	4490	57	0
21	DH	3849	0	3811	44	0
22	DJ	2521	0	2464	25	0
23	DK	1929	0	1928	22	0
24	DT	1912	0	1787	26	0
25	DV	1323	0	1308	17	0
26	DW	1140	0	1117	15	0
27	DX	967	0	956	8	0
28	DY	1295	0	1290	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	F1	6729	0	6773	77	0
30	F4	4382	0	4291	53	0
31	FD	3135	0	3117	39	0
32	FF	3265	0	3204	37	0
33	FG	1359	0	1376	16	0
34	FH	2486	0	2430	34	0
35	FI	2786	0	2712	49	0
36	FK	1699	0	1589	24	0
37	FL	2555	0	2530	45	0
38	FV	1636	0	1567	17	0
39	Fe	1033	0	1004	17	0
40	Ua	282	0	285	11	0
41	Ub	252	0	256	13	0
42	Uc	72	0	76	3	0
43	Ud	354	0	356	12	0
44	Ue	174	0	176	2	0
45	Uf	54	0	56	3	0
46	Ug	1002	0	1026	13	0
47	Uh	1530	0	1557	38	0
48	Ui	192	0	194	9	0
49	Uj	114	0	118	1	0
50	Uk	162	0	164	4	0
51	Ul	84	0	86	0	0
52	Um	66	0	68	7	0
53	Ux	648	0	657	13	0
54	CgA	32	0	12	4	0
55	CgB	1	0	0	0	0
56	F1A	1	0	0	0	0
56	FGA	1	0	0	0	0
56	FLA	1	0	0	0	0
56	FLB	1	0	0	0	0
56	FeA	1	0	0	0	0
57	F1B	26	0	19	2	0
57	FFA	26	0	19	4	0
58	CgC	3	0	0	0	0
All	All	104694	0	101694	1056	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (1056) 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)
8:CC:66:GLU:HG2	39:Fe:12:LEU:HD11	1.35	1.08
18:DE:725:PRO:HG2	43:Ud:28:UNK:HG1	1.48	0.95
35:FI:44:ARG:HH22	52:Um:7:UNK:HG1	1.30	0.95
30:F4:211:TRP:O	30:F4:224:GLY:HA2	1.75	0.86
8:CC:65:PHE:CD1	37:FL:257:PRO:HB3	2.12	0.83
8:CC:58:PHE:HB3	8:CC:72:ILE:HG23	1.58	0.83
16:DB:1013:ARG:HH21	41:Ub:29:UNK:HG1	1.44	0.82
8:CC:66:GLU:HG2	39:Fe:12:LEU:CD1	2.10	0.81
35:FI:44:ARG:NH2	52:Um:7:UNK:HG1	1.95	0.81
47:Uh:1:UNK:HG3	47:Uh:328:UNK:HB1	1.66	0.78
8:CC:58:PHE:CD1	8:CC:72:ILE:CG2	2.66	0.78
8:CC:32:SER:HB3	45:Uf:1:UNK:HG1	1.66	0.78
30:F4:178:TRP:O	30:F4:182:SER:HB3	1.84	0.76
19:DF:224:ARG:HH12	47:Uh:26:UNK:HG2	1.50	0.75
46:Ug:76:UNK:HG3	46:Ug:132:UNK:HB1	1.69	0.74
46:Ug:3:UNK:HG3	46:Ug:4:UNK:HG3	1.70	0.74
22:DJ:31:HIS:CD2	41:Ub:34:UNK:HG2	2.23	0.74
23:DK:2:SER:N	24:DT:160:TYR:HH	1.88	0.71
46:Ug:100:UNK:HB1	46:Ug:121:UNK:HG1	1.73	0.70
22:DJ:31:HIS:HD2	41:Ub:34:UNK:HG2	1.55	0.70
8:CC:58:PHE:CD1	8:CC:72:ILE:HG22	2.28	0.69
23:DK:134:THR:HA	23:DK:139:SER:H	1.59	0.68
15:Ck:582:THR:HA	15:Ck:585:MET:HG2	1.76	0.68
8:CC:74:THR:HG21	37:FL:200:TYR:HA	1.76	0.68
47:Uh:1:UNK:HG1	47:Uh:125:UNK:H2	1.59	0.67
36:FK:127:PRO:HB2	40:Ua:29:UNK:HG1	1.75	0.67
21:DH:63:ASN:HD21	23:DK:132:HIS:HE1	1.43	0.66
47:Uh:278:UNK:HB1	47:Uh:321:UNK:HG3	1.77	0.66
21:DH:413:ASP:HB3	21:DH:416:LEU:HB2	1.78	0.66
34:FH:393:TYR:HA	36:FK:140:SER:HB3	1.77	0.65
10:CJ:457:THR:H	10:CJ:460:HIS:HD2	1.44	0.65
47:Uh:327:UNK:HG1	47:Uh:333:UNK:HB1	1.79	0.65
17:DC:77:ASP:H	17:DC:81:HIS:HD2	1.45	0.64
37:FL:104:GLY:HA3	37:FL:136:ARG:HH12	1.62	0.64
1:CE:159:HIS:H	30:F4:800:ASN:HD21	1.43	0.64
46:Ug:95:UNK:HB1	46:Ug:135:UNK:HG2	1.79	0.64
42:Uc:2:UNK:HG2	45:Uf:6:UNK:HG3	1.79	0.64
4:FJ:290:LEU:HD11	29:F1:159:VAL:HG12	1.80	0.63
13:Cg:109:PHE:HA	54:CgA:1:GTP:HN21	1.62	0.63
10:CJ:246:LYS:HB2	10:CJ:432:HIS:HB2	1.80	0.63
24:DT:35:LYS:HD2	24:DT:219:GLN:HE21	1.63	0.62
18:DE:430:VAL:HG13	18:DE:432:GLU:H	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:DB:655:LEU:HD21	19:DF:561:LEU:HD13	1.82	0.62
17:DC:119:THR:HG23	17:DC:132:SER:HB3	1.80	0.62
35:FI:153:GLN:HE21	35:FI:180:MET:HE3	1.65	0.62
8:CC:65:PHE:CD1	37:FL:257:PRO:CB	2.82	0.62
18:DE:725:PRO:CG	43:Ud:28:UNK:HG1	2.27	0.62
13:Cg:294:GLU:HA	13:Cg:329:PRO:HA	1.81	0.61
39:Fe:107:LEU:HG	39:Fe:115:ARG:HG2	1.81	0.61
8:CC:74:THR:CB	37:FL:200:TYR:HD2	2.13	0.61
16:DB:1014:TYR:HE1	41:Ub:29:UNK:HG2	1.65	0.61
47:Uh:329:UNK:HB2	47:Uh:332:UNK:HG3	1.81	0.61
18:DE:583:ARG:HH21	23:DK:12:ALA:HB2	1.65	0.61
21:DH:160:ASN:HD21	23:DK:124:ALA:HB2	1.65	0.61
30:F4:314:ALA:HB3	30:F4:336:VAL:HG12	1.82	0.61
31:FD:158:PRO:HD2	31:FD:161:LEU:HD12	1.82	0.61
19:DF:390:GLU:HB3	19:DF:476:LEU:HD21	1.82	0.61
26:DW:55:TRP:NE1	26:DW:132:HIS:O	2.32	0.61
30:F4:692:PRO:O	35:FI:44:ARG:NH2	2.34	0.61
8:CC:46:ILE:HG22	8:CC:47:ILE:HG13	1.81	0.61
17:DC:153:ARG:NH2	23:DK:293:ALA:O	2.35	0.60
10:CJ:376:SER:HG	10:CJ:386:GLU:N	1.99	0.60
28:DY:58:THR:HG23	28:DY:99:GLN:HG2	1.83	0.60
32:FF:439:GLY:O	32:FF:443:ASN:ND2	2.35	0.60
35:FI:44:ARG:NH1	52:Um:4:UNK:O	2.34	0.60
57:FFA:1:SAH:SD	57:FFA:1:SAH:N	2.75	0.59
38:FV:121:CYS:HB3	38:FV:128:LEU:HD11	1.84	0.59
18:DE:323:LEU:HD22	18:DE:444:PHE:HB2	1.83	0.59
21:DH:253:SER:HA	21:DH:258:MET:HE1	1.85	0.59
28:DY:76:ARG:HE	28:DY:84:LYS:HD3	1.66	0.59
17:DC:863:LEU:HD22	18:DE:206:LEU:HD12	1.84	0.59
19:DF:224:ARG:NH1	47:Uh:26:UNK:HG2	2.16	0.59
29:F1:794:THR:HG23	29:F1:797:GLU:H	1.67	0.59
46:Ug:26:UNK:HG3	46:Ug:41:UNK:HG3	1.84	0.59
17:DC:953:MET:HE3	17:DC:971:MET:HE1	1.84	0.59
19:DF:105:PRO:HB3	47:Uh:25:UNK:HA	1.83	0.59
10:CJ:800:LEU:HB2	10:CJ:803:ILE:HD12	1.84	0.59
16:DB:961:ALA:HB1	16:DB:964:ARG:HH21	1.68	0.59
17:DC:116:TYR:O	18:DE:150:ARG:NH1	2.35	0.59
19:DF:502:ARG:HH21	19:DF:520:GLN:HA	1.68	0.59
35:FI:26:GLY:HA3	37:FL:233:ASN:HD22	1.67	0.59
20:DG:540:VAL:HG13	20:DG:569:LEU:HD22	1.85	0.58
31:FD:167:CYS:HB3	31:FD:246:PRO:HG2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:DT:200:TRP:HE1	37:FL:290:THR:HG21	1.67	0.58
53:Ux:76:UNK:HG2	53:Ux:89:UNK:HA	1.84	0.58
17:DC:669:LEU:HD11	17:DC:785:TYR:HB3	1.85	0.58
18:DE:326:SER:HA	18:DE:438:PHE:HB3	1.84	0.58
2:CK:54:LEU:HD13	20:DG:190:GLU:HG3	1.86	0.58
35:FI:81:LEU:O	39:Fe:78:ARG:NH2	2.37	0.58
27:DX:86:PRO:HD2	27:DX:135:ALA:HB2	1.84	0.58
32:FF:131:LEU:HB3	32:FF:201:ILE:HG12	1.85	0.58
34:FH:110:ARG:NH2	34:FH:348:VAL:O	2.37	0.58
15:Ck:414:MET:HG2	15:Ck:418:LYS:HZ2	1.69	0.58
15:Ck:679:GLN:HE21	15:Ck:702:ASN:HD21	1.52	0.58
20:DG:200:GLN:HE21	20:DG:234:GLU:HG3	1.68	0.58
20:DG:467:THR:O	20:DG:478:LYS:NZ	2.36	0.57
15:Ck:817:LEU:HD22	15:Ck:836:THR:HG22	1.86	0.57
24:DT:200:TRP:NE1	37:FL:290:THR:HG21	2.19	0.57
16:DB:514:ARG:HH21	16:DB:851:ILE:HG12	1.70	0.57
18:DE:341:GLU:O	18:DE:345:ASN:ND2	2.36	0.57
19:DF:100:LYS:HE3	47:Uh:21:UNK:HB1	1.86	0.57
35:FI:387:GLN:HE22	50:Uk:3:UNK:HA	1.69	0.57
20:DG:215:LEU:HD22	20:DG:224:LEU:HD12	1.85	0.57
32:FF:372:HIS:ND1	32:FF:403:ALA:O	2.37	0.57
16:DB:984:ASP:HA	16:DB:987:GLU:HG3	1.85	0.57
23:DK:20:GLU:OE1	23:DK:154:ARG:NH1	2.37	0.57
32:FF:383:ILE:O	32:FF:387:GLN:NE2	2.38	0.57
34:FH:240:VAL:HG21	38:FV:181:VAL:HG21	1.87	0.57
8:CC:58:PHE:HB3	8:CC:72:ILE:CG2	2.34	0.57
15:Ck:644:HIS:HD2	15:Ck:669:ASN:HD22	1.52	0.57
19:DF:204:ARG:HG2	47:Uh:303:UNK:HB1	1.87	0.57
27:DX:107:LEU:HD22	27:DX:117:VAL:HG22	1.87	0.57
15:Ck:566:ARG:HH22	15:Ck:572:MET:H	1.53	0.56
17:DC:153:ARG:H	17:DC:183:THR:HG21	1.70	0.56
29:F1:404:ARG:NH1	32:FF:193:PHE:O	2.38	0.56
34:FH:108:ARG:NH1	34:FH:347:GLU:O	2.38	0.56
33:FG:34:ARG:NH1	33:FG:36:MET:SD	2.77	0.56
22:DJ:29:HIS:HB2	41:Ub:39:UNK:HB2	1.87	0.56
24:DT:69:ASP:OD1	35:FI:440:ASN:ND2	2.37	0.56
24:DT:208:ARG:HH11	31:FD:148:GLN:HB3	1.71	0.56
29:F1:131:MET:HE3	29:F1:135:MET:HG3	1.87	0.56
47:Uh:104:UNK:HB2	47:Uh:291:UNK:HG3	1.87	0.56
22:DJ:245:VAL:HG13	22:DJ:250:VAL:HG13	1.87	0.56
34:FH:227:PRO:O	34:FH:431:GLN:NE2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:DB:1133:PRO:HA	16:DB:1137:MET:HB3	1.87	0.56
15:Ck:832:THR:HG22	15:Ck:834:MET:H	1.70	0.56
20:DG:476:GLN:HE22	20:DG:560:GLU:H	1.52	0.56
53:Ux:56:UNK:HB2	53:Ux:60:UNK:HB2	1.88	0.56
46:Ug:136:UNK:O	46:Ug:140:UNK:HG3	2.05	0.56
29:F1:316:ARG:NH1	29:F1:335:GLU:OE1	2.39	0.56
19:DF:520:GLN:O	19:DF:531:ARG:NH1	2.38	0.55
37:FL:262:LEU:HB2	37:FL:271:PHE:HB2	1.87	0.55
19:DF:387:VAL:HG11	19:DF:475:TYR:HE2	1.70	0.55
2:CK:29:PRO:HD2	2:CK:32:LEU:HD12	1.89	0.55
33:FG:146:ARG:NH1	38:FV:74:GLY:O	2.40	0.55
9:CI:87:TYR:O	13:Cg:473:ARG:NH1	2.40	0.55
10:CJ:425:ARG:NH1	22:DJ:39:GLU:OE1	2.40	0.55
7:CA:392:U:OP2	26:DW:125:LYS:NZ	2.39	0.55
20:DG:248:LEU:HD11	20:DG:313:SER:HB2	1.89	0.55
30:F4:64:ARG:NH1	30:F4:141:ASP:OD1	2.40	0.55
35:FI:48:PRO:O	39:Fe:52:ARG:NH2	2.38	0.55
43:Ud:2:UNK:O	43:Ud:6:UNK:HG3	2.06	0.55
5:FY:95:ARG:NH1	32:FF:379:GLU:OE2	2.40	0.55
16:DB:544:ARG:NH1	16:DB:572:ASP:OD1	2.39	0.55
16:DB:504:PHE:HA	16:DB:507:LEU:HD12	1.89	0.55
17:DC:681:ARG:HH12	17:DC:749:GLU:HG3	1.72	0.55
29:F1:529:GLU:HG3	57:F1B:1:SAH:H5'1	1.88	0.55
29:F1:810:GLN:HE22	29:F1:814:ARG:HH21	1.55	0.55
30:F4:469:ARG:HH11	34:FH:368:GLY:HA3	1.72	0.55
31:FD:332:CYS:HG	31:FD:336:THR:HG1	1.53	0.55
35:FI:132:ARG:NH2	35:FI:416:GLN:OE1	2.40	0.55
14:CI:39:ARG:NH1	15:Ck:773:ASP:OD2	2.39	0.55
17:DC:270:LEU:HD13	17:DC:435:LEU:HD21	1.88	0.55
21:DH:175:ALA:HB1	21:DH:206:ILE:HD13	1.89	0.55
7:CA:465:U:OP1	9:CI:293:ARG:NH2	2.40	0.55
16:DB:722:ARG:HG2	16:DB:733:HIS:HB2	1.89	0.55
21:DH:114:HIS:ND1	21:DH:124:TYR:OH	2.38	0.55
47:Uh:3:UNK:HG2	47:Uh:329:UNK:HG3	1.90	0.55
47:Uh:108:UNK:HG3	47:Uh:288:UNK:HG1	1.88	0.55
47:Uh:191:UNK:O	47:Uh:195:UNK:HG3	2.07	0.55
10:CJ:234:GLU:OE2	10:CJ:436:ARG:NH1	2.39	0.54
16:DB:1014:TYR:CE1	41:Ub:29:UNK:HG2	2.41	0.54
31:FD:198:PRO:HB3	31:FD:229:ALA:HB1	1.90	0.54
8:CC:43:TRP:HE3	8:CC:68:LEU:HD23	1.72	0.54
10:CJ:567:GLU:O	10:CJ:571:GLN:NE2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:CJ:639:ARG:HB3	10:CJ:644:GLY:HA2	1.89	0.54
21:DH:330:THR:O	21:DH:343:ASN:ND2	2.40	0.54
26:DW:114:LEU:HD22	26:DW:124:LYS:HE3	1.90	0.54
35:FI:151:ARG:NH1	35:FI:377:GLU:OE2	2.41	0.54
30:F4:482:LEU:HB3	30:F4:571:LEU:HD22	1.88	0.54
18:DE:144:PRO:HG2	18:DE:147:MET:HB2	1.90	0.54
24:DT:92:LYS:NZ	24:DT:175:SER:O	2.40	0.54
29:F1:743:GLU:HB2	29:F1:746:HIS:HB2	1.90	0.54
35:FI:67:GLU:OE1	39:Fe:78:ARG:NH1	2.40	0.54
22:DJ:34:LEU:HG	41:Ub:34:UNK:HG3	1.89	0.54
35:FI:415:LEU:HD11	37:FL:18:LEU:HD13	1.90	0.54
37:FL:26:GLU:OE1	37:FL:29:ARG:NH1	2.41	0.54
37:FL:42:ARG:NH1	37:FL:94:ASP:O	2.40	0.54
15:Ck:685:TYR:HA	15:Ck:690:TRP:HE1	1.72	0.54
16:DB:490:ARG:NH2	16:DB:1009:ASP:O	2.40	0.54
10:CJ:263:ASP:OD1	16:DB:1023:ARG:NH2	2.40	0.54
30:F4:261:GLU:HB2	30:F4:578:VAL:HG13	1.88	0.54
8:CC:58:PHE:CD1	8:CC:72:ILE:HG21	2.42	0.54
10:CJ:288:GLN:OE1	21:DH:269:ARG:NH1	2.40	0.54
31:FD:52:ALA:O	31:FD:264:GLN:NE2	2.41	0.54
32:FF:47:ALA:CB	44:Ue:21:UNK:HG1	2.38	0.54
36:FK:132:GLU:OE2	40:Ua:32:UNK:HG3	2.07	0.54
15:Ck:703:ARG:O	15:Ck:759:ASN:ND2	2.40	0.54
30:F4:375:CYS:SG	30:F4:376:ASP:N	2.80	0.54
18:DE:554:LEU:HD11	43:Ud:53:UNK:HG1	1.90	0.53
20:DG:475:GLN:HG2	20:DG:557:GLN:HE21	1.72	0.53
21:DH:303:GLU:OE2	21:DH:307:ARG:NH1	2.40	0.53
22:DJ:132:ARG:NH1	22:DJ:171:LYS:O	2.41	0.53
22:DJ:355:ASP:OD1	22:DJ:355:ASP:N	2.42	0.53
28:DY:145:ARG:O	28:DY:148:ARG:NH2	2.42	0.53
30:F4:233:THR:HG21	30:F4:348:ASN:HD22	1.72	0.53
32:FF:344:LEU:O	32:FF:402:ARG:NH1	2.41	0.53
6:Fa:162:LEU:HB3	28:DY:83:TYR:HD2	1.72	0.53
13:Cg:296:HIS:HD2	27:DX:129:PRO:HD2	1.73	0.53
15:Ck:113:ASN:O	15:Ck:140:ARG:NH2	2.41	0.53
16:DB:748:HIS:HD2	16:DB:751:THR:HG22	1.73	0.53
20:DG:211:TYR:OH	20:DG:234:GLU:OE1	2.26	0.53
9:CI:250:ASN:ND2	9:CI:276:ASP:OD2	2.41	0.53
21:DH:507:ARG:HE	21:DH:511:VAL:HG21	1.74	0.53
10:CJ:185:ASP:O	20:DG:133:ARG:NH2	2.41	0.53
16:DB:546:ARG:NH1	16:DB:875:GLY:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:DY:32:TRP:O	28:DY:37:ARG:NH1	2.40	0.53
32:FF:217:ARG:NH2	32:FF:232:ARG:O	2.41	0.53
35:FI:27:ALA:HB1	52:Um:3:UNK:HG1	1.89	0.53
35:FI:368:ARG:NH1	35:FI:372:GLU:OE1	2.41	0.53
47:Uh:71:UNK:HG2	47:Uh:281:UNK:H2	1.74	0.53
17:DC:968:THR:HB	17:DC:971:MET:HB2	1.89	0.53
30:F4:107:GLY:HA2	30:F4:608:SER:HB3	1.90	0.53
36:FK:184:ARG:HB3	38:FV:185:ARG:HH21	1.72	0.53
38:FV:129:VAL:HG21	38:FV:165:ARG:HD3	1.90	0.53
29:F1:631:HIS:HB3	29:F1:632:MET:HE2	1.91	0.53
13:Cg:329:PRO:HG2	13:Cg:332:ARG:HG2	1.90	0.53
14:Ci:101:LEU:HD13	15:Ck:697:MET:HE1	1.91	0.53
15:Ck:197:GLU:OE1	15:Ck:249:LYS:NZ	2.42	0.53
15:Ck:552:LEU:HD23	15:Ck:561:SER:HB2	1.91	0.53
16:DB:1074:SER:O	16:DB:1077:ARG:NH1	2.41	0.53
17:DC:147:ARG:NH2	23:DK:282:GLU:OE1	2.42	0.53
34:FH:449:VAL:HG11	38:FV:117:ILE:HD11	1.91	0.53
16:DB:557:ALA:O	19:DF:512:ASN:ND2	2.41	0.53
35:FI:200:ARG:NH1	35:FI:206:ASP:OD2	2.42	0.53
10:CJ:475:VAL:HG11	10:CJ:669:PRO:HB2	1.91	0.53
15:Ck:564:LEU:HA	15:Ck:567:LYS:HD2	1.89	0.53
17:DC:172:SER:OG	17:DC:511:ARG:NH1	2.41	0.53
23:DK:149:ASP:OD2	23:DK:149:ASP:N	2.41	0.53
26:DW:159:THR:HA	26:DW:164:ASN:HD21	1.74	0.53
32:FF:309:ARG:NH2	32:FF:355:ARG:O	2.41	0.53
35:FI:136:SER:HB2	35:FI:138:ARG:HE	1.74	0.53
39:Fe:85:CYS:SG	39:Fe:86:ALA:N	2.75	0.53
17:DC:791:ALA:HB3	17:DC:806:SER:HB3	1.90	0.53
30:F4:201:SER:HB2	30:F4:231:HIS:HA	1.90	0.53
34:FH:419:VAL:HG13	34:FH:423:LEU:HD23	1.91	0.53
35:FI:114:SER:HB2	37:FL:197:ARG:HE	1.74	0.53
12:CS:135:ASN:HB3	12:CS:143:LEU:HD21	1.91	0.52
14:Ci:34:ARG:NH1	14:Ci:43:GLU:OE1	2.42	0.52
29:F1:114:GLN:NE2	29:F1:771:PHE:O	2.43	0.52
30:F4:62:SER:OG	30:F4:63:ILE:N	2.41	0.52
36:FK:312:ASN:HB2	38:FV:149:ALA:HB2	1.90	0.52
47:Uh:80:UNK:HA	47:Uh:83:UNK:HG3	1.92	0.52
9:CI:46:ARG:NH2	13:Cg:74:ILE:O	2.42	0.52
9:CI:292:VAL:HG21	9:CI:408:ILE:HA	1.90	0.52
15:Ck:135:ASN:ND2	15:Ck:137:THR:O	2.42	0.52
20:DG:102:MET:HE1	20:DG:134:PRO:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:DH:295:ASP:N	21:DH:295:ASP:OD1	2.43	0.52
20:DG:401:CYS:HB2	20:DG:458:LEU:HB2	1.91	0.52
23:DK:220:PRO:HG2	23:DK:223:ALA:HB2	1.90	0.52
29:F1:781:ALA:HB3	53:Ux:63:UNK:HG3	1.91	0.52
33:FG:163:ASP:HB3	33:FG:172:ALA:H	1.73	0.52
14:CI:153:ARG:NH2	36:FK:182:ASP:OD2	2.42	0.52
21:DH:494:PRO:HB2	21:DH:497:MET:HG2	1.92	0.52
31:FD:422:PHE:CE1	48:Ui:9:UNK:HG2	2.44	0.52
33:FG:16:ARG:H	37:FL:335:GLN:HE22	1.57	0.52
36:FK:241:ASP:N	36:FK:241:ASP:OD1	2.41	0.52
9:CI:98:TYR:HB2	10:CJ:186:VAL:HG11	1.91	0.52
11:CN:165:ARG:NH2	16:DB:1088:TYR:OH	2.42	0.52
15:Ck:384:LEU:O	15:Ck:415:ASN:ND2	2.43	0.52
16:DB:982:PHE:O	16:DB:985:LYS:NZ	2.43	0.52
21:DH:521:ILE:HD12	37:FL:96:PRO:HD2	1.89	0.52
29:F1:165:ARG:NH1	29:F1:248:TYR:OH	2.43	0.52
29:F1:442:ASP:OD1	29:F1:442:ASP:N	2.41	0.52
13:Cg:65:THR:HG22	13:Cg:67:THR:H	1.75	0.52
30:F4:183:LEU:HD13	30:F4:198:LEU:HD11	1.91	0.52
8:CC:31:ASN:O	37:FL:173:GLN:NE2	2.43	0.52
13:Cg:205:ARG:HH21	13:Cg:259:ILE:HG12	1.75	0.52
29:F1:320:GLN:O	29:F1:323:GLN:NE2	2.42	0.52
29:F1:821:ARG:NH2	29:F1:882:GLY:O	2.43	0.52
30:F4:109:ALA:O	30:F4:614:ARG:NH2	2.43	0.52
31:FD:74:ARG:NH2	31:FD:78:TYR:OH	2.43	0.52
33:FG:117:ALA:HB1	38:FV:163:ASN:HD22	1.74	0.52
9:CI:71:GLU:O	26:DW:99:HIS:NE2	2.43	0.52
10:CJ:551:ARG:HH22	10:CJ:590:PHE:HB3	1.75	0.52
14:CI:96:ASN:HD21	15:Ck:697:MET:HA	1.75	0.52
16:DB:526:PRO:HB3	16:DB:530:GLU:HB2	1.92	0.52
30:F4:775:THR:O	30:F4:779:LYS:NZ	2.42	0.52
37:FL:176:LYS:NZ	37:FL:188:MET:O	2.43	0.52
37:FL:197:ARG:NH1	37:FL:202:PRO:O	2.42	0.52
9:CI:61:ARG:NH2	13:Cg:36:ALA:O	2.43	0.52
9:CI:410:LEU:HD22	9:CI:415:LEU:HD12	1.91	0.52
15:Ck:724:PHE:O	15:Ck:778:GLN:NE2	2.43	0.52
31:FD:326:ARG:HE	48:Ui:26:UNK:HG1	1.74	0.52
38:FV:51:SER:HB3	38:FV:58:VAL:HB	1.92	0.52
16:DB:960:ALA:O	16:DB:963:ARG:NH1	2.42	0.51
25:DV:48:HIS:O	25:DV:61:ARG:NH1	2.43	0.51
29:F1:598:PRO:HB2	29:F1:843:LEU:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CK:56:GLN:HE21	13:Cg:488:ARG:HH12	1.58	0.51
4:FJ:279:LEU:HD23	26:DW:116:LEU:HD22	1.92	0.51
6:Fa:140:ALA:O	6:Fa:146:ARG:NH1	2.43	0.51
17:DC:372:ASP:OD1	17:DC:372:ASP:N	2.44	0.51
29:F1:323:GLN:H	29:F1:332:GLN:HE22	1.57	0.51
47:Uh:127:UNK:HB2	53:Ux:121:UNK:HG2	1.91	0.51
17:DC:790:ARG:HG2	17:DC:807:VAL:HG22	1.91	0.51
18:DE:526:SER:O	18:DE:530:TRP:N	2.44	0.51
20:DG:624:ARG:HG2	25:DV:183:LEU:HD12	1.92	0.51
21:DH:353:VAL:HA	21:DH:356:GLN:HE21	1.75	0.51
24:DT:20:VAL:O	33:FG:67:ARG:NE	2.42	0.51
29:F1:80:ARG:NH2	29:F1:147:GLU:OE1	2.43	0.51
29:F1:123:ASP:O	29:F1:277:LYS:NZ	2.42	0.51
16:DB:706:GLU:OE2	18:DE:634:ARG:NH2	2.44	0.51
4:FJ:293:ARG:NH1	29:F1:156:ARG:O	2.44	0.51
16:DB:495:LEU:HD13	16:DB:964:ARG:HD2	1.91	0.51
17:DC:178:ARG:NH2	31:FD:397:ASP:OD1	2.43	0.51
18:DE:584:ASP:OD1	18:DE:584:ASP:N	2.43	0.51
19:DF:237:LEU:HB3	19:DF:253:ILE:HD13	1.91	0.51
26:DW:107:ASP:OD2	28:DY:97:ARG:NH2	2.43	0.51
36:FK:174:ASP:O	36:FK:184:ARG:NH2	2.44	0.51
10:CJ:128:LYS:NZ	16:DB:891:GLN:O	2.44	0.51
13:Cg:260:ASP:OD1	13:Cg:260:ASP:N	2.37	0.51
15:Ck:822:ARG:NH1	15:Ck:823:ASP:OD1	2.43	0.51
20:DG:470:SER:OG	20:DG:471:GLU:N	2.44	0.51
7:CA:515:U:O2	26:DW:126:ARG:NH1	2.44	0.51
9:CI:333:ILE:HG23	9:CI:370:ALA:HB3	1.92	0.51
13:Cg:150:PRO:O	13:Cg:155:LYS:NZ	2.44	0.51
21:DH:305:VAL:HG22	21:DH:360:LEU:HD11	1.93	0.51
29:F1:347:ASN:O	29:F1:350:LYS:NZ	2.42	0.51
34:FH:292:ARG:NH1	36:FK:176:SER:O	2.43	0.51
39:Fe:41:GLU:HA	39:Fe:46:ILE:HD11	1.92	0.51
29:F1:611:MET:HA	29:F1:824:ARG:HH21	1.75	0.51
47:Uh:19:UNK:HB1	47:Uh:21:UNK:HG3	1.92	0.51
50:Uk:7:UNK:HB1	50:Uk:9:UNK:HG2	1.92	0.51
5:FY:53:LEU:HB3	32:FF:37:LEU:HD13	1.93	0.51
10:CJ:488:SER:H	10:CJ:491:ALA:HB3	1.74	0.51
10:CJ:810:ARG:NH2	15:Ck:702:ASN:OD1	2.44	0.51
13:Cg:415:PHE:O	13:Cg:419:SER:HB2	2.10	0.51
17:DC:258:ILE:HD13	17:DC:387:ARG:HH12	1.76	0.51
27:DX:73:THR:O	27:DX:111:ASN:ND2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:FG:67:ARG:NH1	34:FH:238:PRO:O	2.44	0.51
8:CC:67:TYR:O	8:CC:69:ILE:HG13	2.11	0.51
10:CJ:543:THR:HG22	10:CJ:545:SER:H	1.76	0.51
13:Cg:110:LEU:H	54:CgA:1:GTP:HN1	1.58	0.51
15:Ck:102:PRO:HD3	20:DG:22:GLN:HG2	1.93	0.51
16:DB:1113:GLN:O	16:DB:1116:ARG:NH1	2.43	0.51
27:DX:71:PHE:O	27:DX:76:ARG:NH2	2.44	0.51
30:F4:67:ARG:NH1	30:F4:452:PHE:O	2.43	0.51
47:Uh:128:UNK:HG2	47:Uh:324:UNK:H	1.74	0.51
9:CI:422:ARG:NH2	21:DH:499:GLU:OE1	2.44	0.50
10:CJ:336:SER:OG	10:CJ:340:ARG:NH1	2.44	0.50
13:Cg:99:GLN:NE2	54:CgA:1:GTP:O3'	2.44	0.50
18:DE:613:ILE:HG22	23:DK:108:LYS:HE3	1.92	0.50
30:F4:151:ARG:NH2	30:F4:168:ASP:OD2	2.45	0.50
34:FH:330:ARG:NH1	38:FV:154:GLU:O	2.44	0.50
50:Uk:14:UNK:HG2	50:Uk:16:UNK:HB1	1.92	0.50
21:DH:226:PRO:HB3	21:DH:248:VAL:HG13	1.93	0.50
34:FH:401:LEU:O	35:FI:11:ARG:NH1	2.44	0.50
36:FK:140:SER:HB2	36:FK:170:LEU:HD12	1.94	0.50
36:FK:162:GLU:OE2	36:FK:337:ARG:NH1	2.43	0.50
43:Ud:28:UNK:HG2	43:Ud:29:UNK:N	2.27	0.50
10:CJ:693:LEU:HD21	10:CJ:696:ILE:HD11	1.93	0.50
11:CN:165:ARG:NH1	15:Ck:751:ASP:OD2	2.44	0.50
21:DH:510:GLY:HA3	21:DH:516:ILE:HD12	1.92	0.50
25:DV:51:ASN:ND2	28:DY:11:THR:OG1	2.42	0.50
46:Ug:30:UNK:HG2	46:Ug:32:UNK:HG2	1.93	0.50
13:Cg:102:PRO:HG2	13:Cg:105:HIS:HB2	1.93	0.50
13:Cg:279:LEU:O	13:Cg:350:ASN:ND2	2.44	0.50
17:DC:413:LEU:HD11	17:DC:449:VAL:HG13	1.94	0.50
19:DF:349:ASP:OD1	19:DF:349:ASP:N	2.44	0.50
30:F4:437:LEU:HA	30:F4:524:ALA:O	2.11	0.50
32:FF:232:ARG:NH1	32:FF:238:GLY:O	2.44	0.50
34:FH:420:SER:OG	34:FH:421:ASP:N	2.44	0.50
47:Uh:2:UNK:HB2	47:Uh:329:UNK:HG1	1.93	0.50
10:CJ:118:MET:HE1	10:CJ:208:PHE:HZ	1.77	0.50
16:DB:493:ARG:NH2	20:DG:29:ASP:OD2	2.43	0.50
16:DB:1077:ARG:NE	16:DB:1081:TYR:O	2.39	0.50
17:DC:973:PRO:HB3	23:DK:244:LEU:HD21	1.94	0.50
26:DW:51:GLY:O	28:DY:126:LYS:NZ	2.43	0.50
29:F1:471:ARG:O	29:F1:474:ARG:NH1	2.45	0.50
29:F1:824:ARG:HB2	29:F1:835:ASP:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:FL:75:GLN:HE22	37:FL:91:ALA:HA	1.77	0.50
8:CC:58:PHE:CG	8:CC:72:ILE:CG2	2.94	0.50
13:Cg:159:MET:HE3	13:Cg:356:CYS:HB3	1.93	0.50
16:DB:516:VAL:HB	16:DB:522:MET:HE2	1.93	0.50
17:DC:861:VAL:HG12	17:DC:888:LEU:HD21	1.93	0.50
21:DH:145:ALA:HB1	21:DH:151:LEU:HB3	1.94	0.50
25:DV:58:ALA:HA	25:DV:61:ARG:HD2	1.92	0.50
29:F1:103:ARG:HH11	29:F1:344:GLN:HE22	1.60	0.50
34:FH:307:LEU:HA	34:FH:311:ALA:HB2	1.93	0.50
15:Ck:834:MET:HG2	15:Ck:838:LEU:HD22	1.94	0.50
18:DE:313:ARG:NH1	18:DE:529:ASP:OD2	2.44	0.50
30:F4:442:LEU:O	30:F4:468:ARG:NH1	2.44	0.50
32:FF:208:SER:HB3	57:FFA:1:SAH:H5'1	1.93	0.50
3:Cn:158:PRO:HD2	29:F1:232:GLN:HE21	1.76	0.50
16:DB:975:LYS:HG3	20:DG:92:GLN:HE22	1.77	0.50
8:CC:49:ILE:HG12	35:FI:67:GLU:HG2	1.93	0.50
11:CN:115:TYR:O	11:CN:119:ASN:ND2	2.39	0.50
17:DC:149:ARG:HD2	17:DC:511:ARG:HH21	1.77	0.50
17:DC:965:ASN:ND2	18:DE:559:SER:O	2.44	0.50
29:F1:537:ARG:NH2	29:F1:574:GLU:OE1	2.45	0.50
35:FI:127:VAL:HG22	35:FI:134:VAL:HG12	1.92	0.50
47:Uh:55:UNK:HG1	47:Uh:347:UNK:HB1	1.94	0.50
13:Cg:27:GLU:OE1	13:Cg:56:ARG:NH1	2.45	0.49
13:Cg:276:GLU:O	13:Cg:351:LYS:NZ	2.45	0.49
16:DB:876:LEU:HD12	16:DB:877:PRO:HD2	1.94	0.49
17:DC:951:ASN:ND2	17:DC:978:TYR:OH	2.44	0.49
20:DG:485:MET:HE2	20:DG:543:VAL:HG22	1.94	0.49
22:DJ:34:LEU:N	41:Ub:34:UNK:HG1	2.26	0.49
22:DJ:226:VAL:O	35:FI:444:ARG:NH1	2.45	0.49
31:FD:415:PRO:HB2	31:FD:417:GLU:HG3	1.93	0.49
10:CJ:754:VAL:HG12	25:DV:107:ILE:HG12	1.94	0.49
16:DB:1080:ARG:HE	19:DF:177:ASP:HA	1.78	0.49
20:DG:151:SER:HB3	46:Ug:2:UNK:HG3	1.94	0.49
20:DG:581:VAL:O	20:DG:585:GLN:NE2	2.45	0.49
24:DT:41:TYR:O	24:DT:52:ARG:NH1	2.45	0.49
32:FF:8:HIS:ND1	32:FF:12:GLU:OE2	2.45	0.49
36:FK:146:ARG:NH2	36:FK:337:ARG:O	2.44	0.49
15:Ck:308:ARG:HD3	15:Ck:712:CYS:HB2	1.93	0.49
15:Ck:538:ALA:O	15:Ck:541:ARG:HB2	2.12	0.49
18:DE:566:ARG:NH1	18:DE:567:HIS:O	2.45	0.49
31:FD:270:ARG:O	31:FD:273:THR:OG1	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:CS:83:PHE:HA	16:DB:1117:THR:HA	1.94	0.49
15:Ck:333:SER:OG	15:Ck:590:ARG:NH1	2.46	0.49
16:DB:983:LEU:HD11	20:DG:123:LEU:HD13	1.94	0.49
29:F1:610:ARG:O	29:F1:824:ARG:NH2	2.45	0.49
30:F4:232:ASP:O	30:F4:345:HIS:NE2	2.46	0.49
9:CI:43:SER:OG	13:Cg:75:ASN:ND2	2.43	0.49
11:CN:111:VAL:HG11	11:CN:127:LEU:HD21	1.94	0.49
17:DC:80:LEU:HD21	17:DC:1050:THR:HG22	1.94	0.49
18:DE:583:ARG:NH2	23:DK:8:ASN:O	2.45	0.49
32:FF:193:PHE:HB2	32:FF:343:MET:HE3	1.94	0.49
5:FY:64:THR:OG1	32:FF:376:SER:O	2.28	0.49
7:CA:454:G:O6	7:CA:472:G:O6	2.30	0.49
7:CA:481:A:OP1	37:FL:316:ARG:NH2	2.46	0.49
10:CJ:273:ARG:NH2	10:CJ:342:ASN:OD1	2.42	0.49
14:CI:155:LYS:HE3	33:FG:17:SER:HA	1.93	0.49
17:DC:158:TYR:O	31:FD:270:ARG:NH2	2.44	0.49
23:DK:4:ARG:NH2	24:DT:133:ASP:OD1	2.45	0.49
31:FD:239:MET:HE3	31:FD:284:GLY:HA3	1.94	0.49
33:FG:143:CYS:SG	33:FG:145:ASN:ND2	2.86	0.49
9:CI:35:GLY:HA3	20:DG:625:VAL:HG11	1.92	0.49
11:CN:91:ASN:ND2	11:CN:100:GLY:O	2.45	0.49
17:DC:97:ARG:NH1	17:DC:777:GLY:O	2.46	0.49
18:DE:581:THR:H	18:DE:585:ARG:HB2	1.77	0.49
37:FL:75:GLN:HE21	37:FL:88:LEU:HD22	1.78	0.49
8:CC:45:ASN:OD1	8:CC:45:ASN:N	2.45	0.49
10:CJ:467:ALA:O	16:DB:1097:ARG:NH1	2.42	0.49
18:DE:578:GLN:OE1	24:DT:126:ARG:NH1	2.46	0.49
32:FF:232:ARG:HA	32:FF:327:ASN:HD21	1.76	0.49
37:FL:277:PHE:HB2	37:FL:280:LYS:HG2	1.94	0.49
8:CC:65:PHE:CZ	37:FL:288:TRP:CD1	3.01	0.49
10:CJ:250:GLU:OE2	10:CJ:428:SER:OG	2.31	0.49
13:Cg:43:ARG:HD2	20:DG:303:ARG:HH22	1.77	0.49
13:Cg:103:PRO:HA	13:Cg:107:ARG:HH22	1.78	0.49
15:Ck:133:TRP:HB3	15:Ck:141:LEU:HB2	1.95	0.49
15:Ck:834:MET:HA	15:Ck:838:LEU:HB3	1.94	0.49
21:DH:214:LEU:HD22	21:DH:221:HIS:HB3	1.95	0.49
33:FG:31:SER:OG	33:FG:32:VAL:N	2.45	0.49
8:CC:29:LYS:HG2	45:Uf:4:UNK:HG1	1.94	0.49
8:CC:74:THR:HG21	37:FL:200:TYR:CD2	2.47	0.49
9:CI:345:ASP:OD1	13:Cg:377:ARG:NH1	2.42	0.49
17:DC:1045:GLN:O	17:DC:1049:ASN:ND2	2.36	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:DW:144:PRO:HB2	26:DW:149:VAL:HG11	1.95	0.49
32:FF:392:THR:HG22	32:FF:394:HIS:H	1.78	0.49
34:FH:108:ARG:HH12	34:FH:347:GLU:HB3	1.78	0.49
15:Ck:700:VAL:HG22	15:Ck:754:GLU:HB3	1.94	0.48
20:DG:324:LEU:HD23	20:DG:361:SER:HB2	1.94	0.48
29:F1:86:ILE:HD11	29:F1:137:ALA:HB2	1.94	0.48
30:F4:334:GLN:NE2	30:F4:366:SER:OG	2.45	0.48
16:DB:1070:SER:HB3	16:DB:1074:SER:HB2	1.94	0.48
19:DF:291:TYR:OH	21:DH:366:HIS:NE2	2.36	0.48
31:FD:136:GLU:OE2	31:FD:189:ARG:NH1	2.46	0.48
17:DC:568:ASP:HA	17:DC:571:MET:HE2	1.94	0.48
20:DG:351:GLN:HE21	20:DG:355:ARG:HH21	1.60	0.48
31:FD:53:GLU:OE1	31:FD:315:ARG:NH1	2.42	0.48
35:FI:137:ALA:H	41:Ub:9:UNK:HG2	1.78	0.48
36:FK:177:LEU:HD13	38:FV:181:VAL:HG12	1.94	0.48
7:CA:506:A:H5"	27:DX:156:TYR:HB3	1.96	0.48
10:CJ:766:LYS:NZ	14:CI:47:GLU:O	2.44	0.48
34:FH:112:PRO:HA	34:FH:335:GLU:HA	1.95	0.48
43:Ud:25:UNK:HG2	43:Ud:30:UNK:HB1	1.95	0.48
8:CC:19:LYS:NZ	8:CC:20:PHE:O	2.46	0.48
9:CI:152:GLN:NE2	46:Ug:19:UNK:O	2.46	0.48
10:CJ:324:ARG:HH22	15:Ck:127:TRP:HB2	1.79	0.48
16:DB:525:ARG:NH1	16:DB:957:TYR:O	2.44	0.48
7:CA:488:A:OP2	29:F1:850:ARG:NH1	2.44	0.48
10:CJ:683:ARG:NH1	16:DB:1105:GLY:O	2.42	0.48
14:CI:86:ASP:N	14:CI:86:ASP:OD1	2.45	0.48
29:F1:452:THR:OG1	29:F1:455:GLU:OE2	2.31	0.48
16:DB:733:HIS:HB3	16:DB:800:GLN:HE21	1.79	0.48
16:DB:1095:GLU:HG2	19:DF:111:ALA:HB2	1.95	0.48
34:FH:410:LEU:HD22	34:FH:414:LYS:HE3	1.95	0.48
36:FK:131:TRP:O	40:Ua:29:UNK:HG2	2.13	0.48
7:CA:421:G:OP2	19:DF:166:ARG:NH1	2.43	0.48
8:CC:58:PHE:HD1	8:CC:72:ILE:HG22	1.75	0.48
9:CI:148:LEU:HD13	9:CI:180:ILE:HD13	1.94	0.48
18:DE:697:THR:HG21	23:DK:34:ASN:HB2	1.95	0.48
19:DF:184:VAL:HG11	19:DF:227:THR:HG23	1.95	0.48
21:DH:166:GLN:OE1	23:DK:116:ARG:NH2	2.40	0.48
21:DH:347:LYS:HB3	21:DH:378:SER:HB2	1.95	0.48
29:F1:547:THR:HG21	29:F1:551:LEU:HB2	1.96	0.48
52:Um:6:UNK:HG2	52:Um:8:UNK:HG3	1.96	0.48
20:DG:196:ARG:NH1	20:DG:227:GLU:OE1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:DT:183:LEU:HG	31:FD:156:ALA:HB2	1.95	0.48
31:FD:422:PHE:HE2	48:Ui:13:UNK:HB2	1.79	0.48
10:CJ:237:GLY:O	10:CJ:239:ARG:N	2.47	0.48
16:DB:1010:LYS:O	20:DG:38:ARG:NH2	2.46	0.48
22:DJ:242:LEU:HB3	22:DJ:294:MET:HE2	1.96	0.48
25:DV:40:HIS:HD2	28:DY:16:SER:HB2	1.79	0.48
29:F1:159:VAL:HA	29:F1:162:ILE:HD12	1.96	0.48
47:Uh:273:UNK:HG1	47:Uh:338:UNK:HB1	1.95	0.48
30:F4:350:GLU:OE1	40:Ua:39:UNK:HB1	2.14	0.47
10:CJ:796:ASP:OD2	14:Ci:87:TYR:OH	2.29	0.47
16:DB:1053:ALA:O	22:DJ:46:ARG:NH1	2.42	0.47
17:DC:349:ASP:HB3	17:DC:352:GLU:HB2	1.96	0.47
23:DK:36:ARG:NH2	23:DK:105:GLU:OE1	2.45	0.47
29:F1:507:ARG:NH2	32:FF:328:ASN:OD1	2.47	0.47
29:F1:603:LYS:HG2	29:F1:920:GLN:HB2	1.95	0.47
10:CJ:370:MET:HA	10:CJ:393:GLU:HA	1.96	0.47
16:DB:587:VAL:HG21	16:DB:593:ARG:HG2	1.95	0.47
18:DE:157:ARG:HG3	18:DE:564:ILE:HG23	1.95	0.47
18:DE:198:CYS:HB3	18:DE:202:HIS:HB2	1.95	0.47
18:DE:617:ASP:OD1	23:DK:108:LYS:NZ	2.38	0.47
24:DT:138:SER:OG	24:DT:176:ASP:OD2	2.30	0.47
32:FF:145:LEU:HD23	32:FF:152:THR:HG23	1.96	0.47
37:FL:166:PRO:O	37:FL:169:GLU:HB3	2.14	0.47
52:Um:1:UNK:O	52:Um:5:UNK:HG2	2.14	0.47
10:CJ:263:ASP:O	16:DB:1023:ARG:NH2	2.43	0.47
10:CJ:312:ASP:HB2	15:Ck:638:ARG:HH12	1.78	0.47
16:DB:651:ASN:OD1	16:DB:843:ASN:ND2	2.40	0.47
29:F1:506:LYS:HA	32:FF:238:GLY:HA3	1.96	0.47
35:FI:84:LEU:HD12	39:Fe:75:PRO:HD2	1.96	0.47
8:CC:31:ASN:HD22	35:FI:113:ALA:H	1.62	0.47
15:Ck:116:THR:HG22	19:DF:548:ARG:HG3	1.95	0.47
15:Ck:264:ASN:OD1	15:Ck:267:TYR:N	2.47	0.47
17:DC:346:ASP:OD1	17:DC:346:ASP:N	2.47	0.47
19:DF:230:PRO:HG2	19:DF:233:VAL:HG23	1.96	0.47
35:FI:192:GLU:OE2	35:FI:195:ARG:NH1	2.47	0.47
9:CI:146:ASP:OD1	9:CI:146:ASP:N	2.42	0.47
20:DG:401:CYS:SG	20:DG:402:PHE:N	2.88	0.47
29:F1:761:ARG:HG2	29:F1:895:THR:HG22	1.96	0.47
53:Ux:99:UNK:HG1	53:Ux:102:UNK:HG3	1.96	0.47
7:CA:416:U:O2'	11:CN:19:LYS:NZ	2.43	0.47
11:CN:81:LEU:O	11:CN:83:LYS:NZ	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:DC:367:MET:HB3	17:DC:379:LEU:HB2	1.95	0.47
17:DC:390:GLU:OE1	17:DC:397:TYR:OH	2.31	0.47
17:DC:469:THR:HA	23:DK:290:GLY:HA3	1.96	0.47
18:DE:592:PRO:O	43:Ud:32:UNK:HG1	2.15	0.47
19:DF:169:ARG:O	21:DH:394:ARG:NH1	2.46	0.47
25:DV:60:LEU:HD23	25:DV:82:VAL:HG12	1.95	0.47
30:F4:67:ARG:HH22	30:F4:455:LEU:HD12	1.80	0.47
34:FH:397:TYR:OH	36:FK:178:ASP:OD2	2.32	0.47
47:Uh:105:UNK:HG2	47:Uh:118:UNK:HB2	1.97	0.47
53:Ux:33:UNK:HG1	53:Ux:39:UNK:N	2.30	0.47
53:Ux:42:UNK:O	53:Ux:46:UNK:HG3	2.15	0.47
53:Ux:76:UNK:HG1	53:Ux:87:UNK:HG2	1.97	0.47
9:CI:137:SER:OG	9:CI:139:ASP:OD2	2.32	0.47
13:Cg:70:SER:OG	13:Cg:71:PHE:N	2.47	0.47
16:DB:455:ARG:NH2	21:DH:256:GLY:O	2.48	0.47
17:DC:397:TYR:O	17:DC:403:ARG:NH2	2.47	0.47
20:DG:590:ARG:HH11	20:DG:592:THR:HB	1.80	0.47
37:FL:65:ARG:NH2	37:FL:98:ASP:OD2	2.40	0.47
10:CJ:396:LYS:HD2	10:CJ:809:PRO:HB2	1.96	0.47
13:Cg:37:ILE:HD12	13:Cg:422:LEU:HD13	1.97	0.47
15:Ck:742:GLY:HA2	25:DV:127:THR:HG23	1.96	0.47
18:DE:699:ASN:HD22	18:DE:707:ARG:HH12	1.62	0.47
19:DF:116:ARG:NH1	19:DF:179:TYR:OH	2.48	0.47
31:FD:90:THR:HG23	35:FI:410:ALA:HB1	1.97	0.47
31:FD:111:THR:HG22	39:Fe:3:ARG:HD3	1.97	0.47
53:Ux:116:UNK:O	53:Ux:120:UNK:HG3	2.15	0.47
15:Ck:141:LEU:HD23	15:Ck:262:VAL:HG11	1.96	0.47
8:CC:74:THR:HG21	37:FL:200:TYR:HD2	1.80	0.46
29:F1:741:THR:HG21	29:F1:870:ILE:HG21	1.97	0.46
31:FD:422:PHE:CE2	48:Ui:13:UNK:HB2	2.50	0.46
35:FI:203:LEU:HD11	35:FI:396:GLN:HB3	1.97	0.46
13:Cg:373:VAL:HG11	25:DV:51:ASN:HD22	1.80	0.46
20:DG:166:GLU:OE1	20:DG:207:ARG:NH2	2.46	0.46
29:F1:155:LEU:O	29:F1:159:VAL:HB	2.15	0.46
29:F1:904:ASN:HA	29:F1:907:LEU:HD12	1.98	0.46
34:FH:254:LYS:HB2	34:FH:271:CYS:HB2	1.97	0.46
7:CA:474:U:H5'	21:DH:556:ARG:HH12	1.79	0.46
10:CJ:245:TYR:HB2	10:CJ:403:CYS:HB2	1.97	0.46
10:CJ:502:GLU:OE2	10:CJ:524:THR:OG1	2.33	0.46
15:Ck:708:ARG:HG2	15:Ck:747:LYS:HG3	1.98	0.46
17:DC:386:MET:HE3	17:DC:442:LEU:HD23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:DK:272:GLU:OE1	23:DK:275:ARG:NH2	2.42	0.46
25:DV:41:THR:HG22	28:DY:17:VAL:HB	1.97	0.46
29:F1:524:ALA:O	57:F1B:1:SAH:N	2.48	0.46
29:F1:809:GLN:HA	29:F1:812:VAL:HG12	1.98	0.46
15:Ck:395:MET:HE1	15:Ck:568:LEU:HB3	1.97	0.46
16:DB:881:ARG:HB2	16:DB:935:ASP:HB3	1.98	0.46
19:DF:151:VAL:HB	47:Uh:22:UNK:HB1	1.97	0.46
29:F1:850:ARG:NE	29:F1:868:GLN:OE1	2.47	0.46
30:F4:266:ASN:ND2	30:F4:434:ASP:OD2	2.48	0.46
10:CJ:804:ASN:HD21	11:CN:155:VAL:HG21	1.80	0.46
10:CJ:808:PHE:HZ	15:Ck:697:MET:HG2	1.81	0.46
15:Ck:395:MET:HB3	15:Ck:564:LEU:HD11	1.97	0.46
18:DE:68:PRO:O	18:DE:197:ARG:NH1	2.49	0.46
32:FF:16:VAL:HG12	32:FF:213:GLU:HG2	1.96	0.46
33:FG:89:ASP:H	33:FG:92:GLU:HB2	1.79	0.46
35:FI:329:GLU:HB3	35:FI:355:LEU:HA	1.97	0.46
9:CI:34:ASP:OD1	9:CI:37:ARG:NH2	2.45	0.46
10:CJ:542:LYS:HE3	10:CJ:595:THR:HA	1.97	0.46
16:DB:610:SER:OG	16:DB:639:ASP:OD2	2.34	0.46
17:DC:112:TYR:HB3	17:DC:960:VAL:HG13	1.97	0.46
20:DG:483:THR:HA	20:DG:565:CYS:HB2	1.98	0.46
24:DT:114:LEU:O	24:DT:127:LYS:NZ	2.49	0.46
38:FV:180:SER:O	38:FV:186:GLN:NE2	2.45	0.46
49:Uj:6:UNK:HA	49:Uj:9:UNK:HB2	1.96	0.46
15:Ck:358:LYS:HB2	15:Ck:361:GLN:HG3	1.97	0.46
21:DH:156:LEU:HD13	21:DH:216:THR:HG23	1.97	0.46
21:DH:246:GLU:OE2	21:DH:277:THR:OG1	2.30	0.46
7:CA:427:U:H3'	22:DJ:232:ARG:HD3	1.98	0.46
10:CJ:471:GLN:HG3	10:CJ:672:ARG:HG2	1.97	0.46
14:CI:119:LEU:HD22	21:DH:399:PHE:HD2	1.81	0.46
15:Ck:145:LEU:HD21	15:Ck:323:LEU:HD22	1.97	0.46
17:DC:367:MET:O	17:DC:377:THR:OG1	2.32	0.46
19:DF:359:ARG:HB2	22:DJ:78:ALA:HA	1.97	0.46
21:DH:34:TYR:O	21:DH:398:GLN:NE2	2.49	0.46
22:DJ:29:HIS:CB	41:Ub:39:UNK:HB2	2.45	0.46
32:FF:136:GLY:HA3	57:FFA:1:SAH:HA	1.98	0.46
8:CC:65:PHE:HZ	37:FL:288:TRP:CD1	2.33	0.46
13:Cg:468:ASP:OD1	13:Cg:468:ASP:N	2.42	0.46
18:DE:77:PRO:HA	18:DE:80:LEU:HD12	1.97	0.46
21:DH:515:ASP:O	37:FL:136:ARG:NH1	2.49	0.46
22:DJ:34:LEU:HG	41:Ub:34:UNK:CG	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:CJ:792:HIS:HB3	10:CJ:795:LYS:HB2	1.98	0.46
15:Ck:98:ARG:O	20:DG:15:ARG:NH1	2.42	0.46
16:DB:522:MET:HE3	16:DB:522:MET:HB3	1.85	0.46
29:F1:695:ARG:NH1	40:Ua:14:UNK:HG1	2.31	0.46
30:F4:185:SER:O	30:F4:185:SER:OG	2.31	0.46
32:FF:406:SER:O	32:FF:406:SER:OG	2.32	0.46
34:FH:391:LEU:HD23	36:FK:169:GLN:HE22	1.81	0.46
39:Fe:76:SER:HB3	39:Fe:79:VAL:HG23	1.98	0.46
9:CI:305:ILE:HA	9:CI:323:LEU:O	2.15	0.45
16:DB:484:PHE:O	16:DB:487:ARG:NH2	2.49	0.45
20:DG:444:THR:HG23	20:DG:447:ALA:H	1.81	0.45
29:F1:613:ILE:HG22	29:F1:615:SER:HB3	1.98	0.45
13:Cg:231:LEU:O	13:Cg:239:GLN:NE2	2.49	0.45
16:DB:769:VAL:HG22	16:DB:775:ALA:HA	1.99	0.45
16:DB:882:ARG:NH2	16:DB:925:ASP:OD2	2.44	0.45
16:DB:942:ARG:HH22	16:DB:951:GLY:HA2	1.80	0.45
18:DE:650:HIS:HB2	43:Ud:23:UNK:HG1	1.98	0.45
19:DF:148:PRO:O	47:Uh:22:UNK:HG1	2.16	0.45
34:FH:300:SER:OG	34:FH:301:MET:N	2.49	0.45
4:FJ:289:THR:HG21	29:F1:156:ARG:HE	1.81	0.45
9:CI:312:ALA:HB3	9:CI:317:TYR:HB2	1.97	0.45
21:DH:73:LEU:HD13	21:DH:97:LEU:HD11	1.97	0.45
22:DJ:137:MET:HG2	22:DJ:168:TYR:HE2	1.80	0.45
30:F4:681:SER:OG	37:FL:299:ARG:NH1	2.49	0.45
31:FD:104:HIS:HD1	39:Fe:7:PHE:HB3	1.81	0.45
10:CJ:159:LEU:HD23	10:CJ:162:ILE:HD11	1.98	0.45
11:CN:14:GLY:HA3	11:CN:15:GLN:HA	1.75	0.45
15:Ck:132:TYR:CZ	15:Ck:140:ARG:HG3	2.52	0.45
16:DB:993:ASP:N	16:DB:993:ASP:OD1	2.48	0.45
18:DE:647:LEU:HD22	43:Ud:36:UNK:HG1	1.99	0.45
30:F4:335:GLU:OE1	30:F4:369:THR:OG1	2.30	0.45
34:FH:272:THR:HG22	34:FH:274:GLN:H	1.79	0.45
34:FH:305:GLN:NE2	34:FH:309:GLU:OE1	2.42	0.45
16:DB:690:ARG:HA	16:DB:697:ARG:HH21	1.82	0.45
17:DC:357:GLN:NE2	17:DC:361:ASP:OD1	2.50	0.45
30:F4:422:GLY:O	30:F4:425:THR:OG1	2.30	0.45
17:DC:312:TRP:HA	17:DC:315:LEU:HD13	1.99	0.45
8:CC:58:PHE:CB	8:CC:72:ILE:HG23	2.39	0.45
15:Ck:380:VAL:HG23	15:Ck:565:LEU:HD11	1.99	0.45
16:DB:468:THR:HG22	21:DH:331:PRO:HG2	1.99	0.45
19:DF:196:PHE:HD2	19:DF:199:GLU:H	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:DW:117:PHE:HZ	32:FF:430:THR:HG22	1.81	0.45
41:Ub:27:UNK:HA	41:Ub:30:UNK:HG3	1.98	0.45
47:Uh:40:UNK:H2	47:Uh:125:UNK:HB1	1.82	0.45
7:CA:486:C:OP1	29:F1:831:LYS:NZ	2.47	0.45
11:CN:53:GLU:O	11:CN:64:GLN:NE2	2.48	0.45
13:Cg:304:PHE:HA	27:DX:106:LYS:HE3	1.99	0.45
29:F1:99:TYR:OH	29:F1:344:GLN:NE2	2.50	0.45
35:FI:169:ASN:O	41:Ub:4:UNK:HG1	2.17	0.45
46:Ug:95:UNK:HG1	46:Ug:135:UNK:O	2.17	0.45
47:Uh:195:UNK:HG1	53:Ux:126:UNK:HG1	1.99	0.45
10:CJ:268:LEU:HD21	10:CJ:419:ILE:HD11	1.99	0.45
12:CS:65:ASN:HD22	25:DV:69:LYS:HG3	1.81	0.45
15:Ck:416:ARG:HH22	20:DG:161:ARG:HH21	1.65	0.45
20:DG:80:LEU:HA	20:DG:83:MET:HB3	1.99	0.45
20:DG:183:ARG:NH2	20:DG:300:ASP:OD2	2.50	0.45
29:F1:572:ILE:HG21	29:F1:646:LEU:HD13	1.99	0.45
35:FI:412:ARG:NH2	42:Uc:7:UNK:O	2.49	0.45
47:Uh:131:UNK:HG2	47:Uh:286:UNK:HB1	1.99	0.45
13:Cg:247:CYS:O	13:Cg:251:HIS:ND1	2.47	0.45
16:DB:741:THR:HG23	16:DB:760:LYS:HE3	1.99	0.45
18:DE:303:ASP:OD1	18:DE:303:ASP:N	2.49	0.45
20:DG:288:LEU:HD13	20:DG:329:LEU:HA	1.98	0.45
20:DG:319:SER:O	20:DG:362:SER:OG	2.30	0.45
30:F4:249:LEU:HD13	30:F4:327:LEU:HG	1.99	0.45
7:CA:449:G:H5''	21:DH:538:ARG:HH22	1.81	0.44
10:CJ:271:VAL:HG11	10:CJ:415:ARG:HG2	1.99	0.44
14:Ci:75:ASP:OD1	14:Ci:75:ASP:N	2.50	0.44
15:Ck:617:VAL:HG21	15:Ck:638:ARG:HD2	1.97	0.44
16:DB:610:SER:HB3	16:DB:613:VAL:HG23	1.99	0.44
22:DJ:118:ASP:OD1	22:DJ:147:ARG:NH2	2.44	0.44
33:FG:83:LEU:HG	33:FG:109:LEU:HD21	1.99	0.44
15:Ck:283:GLU:OE2	16:DB:887:SER:N	2.50	0.44
16:DB:1094:ASN:OD1	16:DB:1097:ARG:NH2	2.48	0.44
22:DJ:95:THR:O	22:DJ:131:GLN:NE2	2.46	0.44
29:F1:276:SER:HB2	29:F1:324:GLY:H	1.82	0.44
30:F4:465:ASP:OD2	30:F4:465:ASP:N	2.50	0.44
38:FV:49:LEU:HB2	38:FV:60:VAL:HB	1.99	0.44
10:CJ:773:GLU:HB3	25:DV:100:LYS:HG3	1.99	0.44
15:Ck:573:THR:HA	15:Ck:576:ASP:HB2	1.99	0.44
16:DB:1003:LYS:HE3	16:DB:1003:LYS:HB2	1.73	0.44
17:DC:151:SER:HB3	17:DC:227:GLN:HE22	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:DG:83:MET:HE3	20:DG:83:MET:HB2	1.84	0.44
22:DJ:247:ASN:HB3	22:DJ:250:VAL:HG12	2.00	0.44
29:F1:137:ALA:HA	32:FF:445:PHE:HZ	1.83	0.44
29:F1:472:ARG:HH12	29:F1:474:ARG:HH22	1.64	0.44
32:FF:134:THR:OG1	57:FFA:1:SAH:O4'	2.34	0.44
34:FH:252:VAL:HG13	34:FH:280:MET:HB3	2.00	0.44
9:CI:40:TRP:NE1	10:CJ:159:LEU:O	2.51	0.44
9:CI:326:ASN:ND2	9:CI:369:ASP:OD2	2.50	0.44
10:CJ:791:HIS:HD2	14:CI:81:GLY:HA2	1.81	0.44
16:DB:983:LEU:HD13	20:DG:84:LEU:HD22	1.99	0.44
20:DG:83:MET:HE1	20:DG:108:ARG:HD2	1.98	0.44
30:F4:417:PRO:HA	40:Ua:26:UNK:HG1	1.99	0.44
31:FD:38:PRO:O	35:FI:337:TYR:OH	2.34	0.44
16:DB:554:GLU:OE2	16:DB:899:ARG:NH2	2.40	0.44
19:DF:553:THR:OG1	19:DF:554:TYR:N	2.51	0.44
24:DT:18:MET:SD	24:DT:208:ARG:NH2	2.90	0.44
29:F1:337:ARG:HH12	29:F1:461:GLU:HG2	1.83	0.44
30:F4:699:ASP:O	39:Fe:44:LYS:NZ	2.51	0.44
31:FD:184:GLN:HE21	34:FH:105:LEU:HD21	1.82	0.44
31:FD:248:GLU:HA	31:FD:251:ASP:HB3	1.98	0.44
4:FJ:301:ASP:OD1	29:F1:164:TYR:OH	2.34	0.44
8:CC:14:GLN:OE1	24:DT:127:LYS:NZ	2.50	0.44
10:CJ:729:ASP:OD1	10:CJ:729:ASP:N	2.50	0.44
17:DC:266:PHE:O	17:DC:271:SER:OG	2.32	0.44
19:DF:154:ASN:O	19:DF:182:ARG:NH1	2.50	0.44
26:DW:138:ALA:HA	26:DW:145:ARG:HH12	1.83	0.44
37:FL:237:SER:O	37:FL:237:SER:OG	2.35	0.44
5:FY:16:PRO:HD2	32:FF:413:THR:HA	1.98	0.44
10:CJ:478:LEU:HD21	19:DF:214:HIS:HD2	1.83	0.44
12:CS:90:ILE:HB	19:DF:94:ASP:HA	2.00	0.44
15:Ck:341:LEU:O	15:Ck:345:SER:OG	2.34	0.44
16:DB:778:LYS:HE2	16:DB:781:GLY:H	1.83	0.44
21:DH:195:TYR:HA	21:DH:198:GLN:HE21	1.83	0.44
21:DH:308:ARG:HH22	21:DH:359:GLU:HG2	1.82	0.44
17:DC:63:ASP:OD1	17:DC:63:ASP:N	2.44	0.44
19:DF:435:THR:HG22	19:DF:437:GLU:H	1.83	0.44
30:F4:248:LEU:HD13	30:F4:631:LEU:HD11	2.00	0.44
31:FD:66:LEU:HD22	35:FI:355:LEU:HD11	1.98	0.44
34:FH:322:GLU:HG2	36:FK:310:ILE:HD11	1.99	0.44
10:CJ:496:LEU:HD13	10:CJ:521:VAL:HG13	1.99	0.44
13:Cg:147:VAL:H	13:Cg:356:CYS:HA	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Ck:660:PRO:HG3	16:DB:1068:GLY:HA2	2.00	0.44
16:DB:559:GLU:OE2	16:DB:567:ARG:NE	2.47	0.44
17:DC:163:ASN:HB2	24:DT:121:ASP:HA	2.00	0.44
18:DE:658:ASN:HD22	18:DE:661:LYS:HD2	1.83	0.44
22:DJ:224:LEU:HD11	35:FI:434:VAL:HB	1.99	0.44
24:DT:17:HIS:HB2	24:DT:192:GLN:HG2	2.00	0.44
29:F1:793:ILE:HG23	29:F1:797:GLU:HG2	2.00	0.44
30:F4:204:ARG:NH2	30:F4:230:TRP:O	2.47	0.44
30:F4:486:LEU:HD13	30:F4:572:GLU:HG2	2.00	0.44
9:CI:14:ARG:NH1	20:DG:296:ASP:OD2	2.48	0.43
10:CJ:783:ILE:HD13	14:CI:53:TRP:HZ3	1.82	0.43
30:F4:369:THR:HG22	40:Ua:42:UNK:HA	2.00	0.43
30:F4:687:TRP:O	30:F4:691:THR:OG1	2.35	0.43
35:FI:27:ALA:CB	52:Um:3:UNK:HG1	2.48	0.43
35:FI:105:GLU:HG3	39:Fe:9:PRO:HB3	2.00	0.43
37:FL:89:VAL:HG23	37:FL:114:PHE:HD2	1.83	0.43
47:Uh:75:UNK:HA	47:Uh:78:UNK:HG3	2.00	0.43
10:CJ:434:ILE:HD13	15:Ck:708:ARG:HH12	1.84	0.43
10:CJ:775:ASP:OD1	25:DV:56:ARG:NH2	2.50	0.43
13:Cg:197:PHE:HE1	15:Ck:810:ILE:HD13	1.83	0.43
16:DB:611:PRO:HA	16:DB:614:VAL:HG22	2.00	0.43
20:DG:55:PRO:HA	20:DG:58:TRP:HB2	2.00	0.43
29:F1:112:MET:HA	29:F1:115:TRP:HD1	1.83	0.43
29:F1:361:LEU:HD22	29:F1:364:ARG:HH21	1.83	0.43
47:Uh:38:UNK:HG3	47:Uh:39:UNK:HG3	2.00	0.43
47:Uh:71:UNK:HG2	47:Uh:281:UNK:N	2.33	0.43
7:CA:442:A:H4'	7:CA:485:U:H5'	2.00	0.43
11:CN:73:CYS:O	11:CN:77:ASN:ND2	2.50	0.43
16:DB:1098:ASP:HB3	47:Uh:26:UNK:HG1	2.00	0.43
18:DE:292:TYR:HD1	18:DE:396:PRO:HG2	1.83	0.43
19:DF:490:ASN:HA	19:DF:493:MET:HG2	1.99	0.43
10:CJ:130:ARG:NH2	15:Ck:308:ARG:O	2.49	0.43
10:CJ:369:ARG:HH22	11:CN:109:PRO:HD2	1.82	0.43
12:CS:51:PRO:HG2	12:CS:54:ARG:HB2	1.99	0.43
16:DB:542:GLN:HE22	16:DB:941:ARG:HH12	1.67	0.43
16:DB:879:ARG:NH1	16:DB:897:PRO:O	2.52	0.43
24:DT:107:GLU:HB3	31:FD:262:LEU:HD21	1.99	0.43
28:DY:15:SER:HA	28:DY:123:ASN:HB2	2.00	0.43
30:F4:178:TRP:NE1	30:F4:201:SER:OG	2.47	0.43
30:F4:685:HIS:HA	30:F4:690:MET:HE3	1.99	0.43
36:FK:265:THR:OG1	36:FK:306:ARG:NH2	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:CI:1:MET:HG2	20:DG:523:LEU:HA	2.01	0.43
9:CI:194:THR:HG23	9:CI:195:ILE:HG13	2.00	0.43
10:CJ:140:ARG:HD2	10:CJ:215:TRP:CD1	2.54	0.43
12:CS:108:LEU:O	12:CS:112:THR:OG1	2.35	0.43
15:Ck:382:GLU:O	15:Ck:386:ASN:ND2	2.51	0.43
17:DC:609:VAL:HG21	17:DC:618:ARG:HD2	2.00	0.43
18:DE:186:ARG:NE	18:DE:426:PHE:O	2.41	0.43
38:FV:60:VAL:HG21	38:FV:234:LEU:HD11	2.00	0.43
47:Uh:1:UNK:HG1	47:Uh:125:UNK:N	2.31	0.43
6:Fa:142:PHE:HE2	9:CI:109:LEU:HG	1.83	0.43
7:CA:465:U:OP2	9:CI:407:ARG:NH2	2.43	0.43
9:CI:110:ARG:HH21	20:DG:143:HIS:HD2	1.66	0.43
30:F4:264:ILE:HD12	30:F4:267:LYS:HE2	2.00	0.43
32:FF:190:LYS:HB2	32:FF:339:ASN:HB3	2.00	0.43
34:FH:330:ARG:HA	34:FH:330:ARG:HD2	1.88	0.43
47:Uh:43:UNK:HG1	47:Uh:325:UNK:HB1	2.01	0.43
12:CS:108:LEU:HD21	47:Uh:13:UNK:HG1	2.01	0.43
19:DF:202:LEU:HB3	19:DF:203:MET:HE2	2.00	0.43
32:FF:242:LEU:O	32:FF:246:ASN:ND2	2.52	0.43
36:FK:125:PRO:HA	36:FK:126:PRO:HD3	1.86	0.43
36:FK:165:THR:HB	36:FK:193:PHE:HB2	2.00	0.43
37:FL:177:ARG:O	37:FL:180:GLU:HB2	2.19	0.43
1:CE:149:MET:HE3	1:CE:149:MET:HB2	1.93	0.43
9:CI:312:ALA:HB1	9:CI:386:ILE:HG22	2.00	0.43
10:CJ:141:ASP:O	10:CJ:145:THR:OG1	2.34	0.43
10:CJ:270:ASP:OD1	10:CJ:273:ARG:NH1	2.52	0.43
12:CS:117:VAL:HB	12:CS:128:PHE:HB2	2.01	0.43
19:DF:187:ASN:HD22	19:DF:191:THR:HG23	1.84	0.43
20:DG:97:VAL:HG12	20:DG:132:ALA:HB2	1.99	0.43
21:DH:37:SER:HB2	21:DH:381:LYS:HA	2.00	0.43
28:DY:20:PRO:HA	28:DY:21:PRO:HD3	1.94	0.43
28:DY:62:GLN:HA	28:DY:65:LEU:HB2	2.00	0.43
31:FD:328:LYS:HE3	48:Ui:23:UNK:HG1	2.01	0.43
9:CI:379:MET:HE3	9:CI:379:MET:HB2	1.87	0.43
10:CJ:181:GLU:HG2	10:CJ:192:ILE:HD11	2.00	0.43
13:Cg:184:HIS:HA	13:Cg:296:HIS:ND1	2.33	0.43
13:Cg:210:TYR:HA	13:Cg:213:VAL:HG22	1.99	0.43
18:DE:194:HIS:HA	18:DE:423:PHE:HE2	1.84	0.43
19:DF:275:MET:O	19:DF:279:ILE:HG12	2.19	0.43
31:FD:326:ARG:NE	48:Ui:26:UNK:HG1	2.34	0.43
34:FH:308:VAL:HG13	34:FH:309:GLU:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:FI:404:ASP:OD2	42:Uc:4:UNK:N	2.51	0.43
37:FL:166:PRO:HG3	37:FL:227:LEU:HD22	2.01	0.43
7:CA:393:U:H2'	7:CA:394:A:C8	2.54	0.43
24:DT:27:ARG:H	37:FL:349:ASN:HD21	1.67	0.43
26:DW:93:HIS:O	26:DW:97:SER:OG	2.31	0.43
31:FD:240:GLN:HG2	31:FD:287:VAL:HB	2.00	0.43
31:FD:327:GLU:OE2	31:FD:331:ARG:NH2	2.42	0.43
35:FI:53:GLU:OE2	39:Fe:52:ARG:NH1	2.52	0.43
38:FV:261:MET:HE2	38:FV:261:MET:HB3	1.86	0.43
10:CJ:364:LEU:HB3	10:CJ:398:PHE:HB2	2.01	0.42
18:DE:40:ASN:O	18:DE:79:TYR:OH	2.36	0.42
22:DJ:133:CYS:O	22:DJ:168:TYR:OH	2.33	0.42
26:DW:111:LYS:HE2	26:DW:131:TRP:HZ2	1.83	0.42
29:F1:863:SER:OG	29:F1:864:THR:N	2.52	0.42
30:F4:593:ASP:N	30:F4:593:ASP:OD1	2.47	0.42
31:FD:109:TYR:OH	35:FI:404:ASP:OD1	2.32	0.42
34:FH:91:ASP:HB3	34:FH:98:ALA:HB2	2.01	0.42
37:FL:249:TYR:HA	37:FL:261:MET:O	2.19	0.42
43:Ud:33:UNK:O	43:Ud:37:UNK:N	2.52	0.42
43:Ud:49:UNK:O	43:Ud:53:UNK:HG2	2.18	0.42
16:DB:1102:TYR:OH	19:DF:100:LYS:O	2.33	0.42
19:DF:448:GLY:H	19:DF:489:ARG:HH12	1.67	0.42
22:DJ:40:ARG:HD3	22:DJ:40:ARG:HA	1.91	0.42
43:Ud:8:UNK:HA	43:Ud:11:UNK:HG3	1.99	0.42
50:Uk:16:UNK:HG3	50:Uk:18:UNK:HG3	2.01	0.42
7:CA:469:A:H2'	7:CA:470:G:C8	2.54	0.42
10:CJ:144:LEU:HD22	10:CJ:214:ASP:HB3	2.01	0.42
10:CJ:235:GLU:HG3	15:Ck:310:ASP:HB3	2.01	0.42
17:DC:788:LEU:HD11	17:DC:807:VAL:HG13	2.01	0.42
18:DE:441:ALA:HA	18:DE:444:PHE:HB3	2.01	0.42
20:DG:63:HIS:ND1	20:DG:94:GLY:O	2.53	0.42
32:FF:47:ALA:HB2	44:Ue:21:UNK:HG1	2.02	0.42
10:CJ:340:ARG:HH21	10:CJ:358:TRP:HD1	1.66	0.42
10:CJ:611:GLU:OE2	10:CJ:665:ARG:NH1	2.50	0.42
17:DC:313:THR:O	17:DC:320:ARG:NH2	2.47	0.42
18:DE:246:ILE:HD11	18:DE:420:VAL:HA	2.02	0.42
18:DE:703:GLN:HA	18:DE:706:ARG:HG2	2.01	0.42
30:F4:235:CYS:SG	30:F4:321:SER:OG	2.71	0.42
30:F4:377:ILE:H	30:F4:377:ILE:HG13	1.56	0.42
30:F4:469:ARG:HD2	34:FH:368:GLY:HA3	2.01	0.42
32:FF:124:ARG:HE	32:FF:127:SER:HB3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:FL:259:HIS:CE1	37:FL:274:ASP:H	2.37	0.42
8:CC:28:ASP:OD2	8:CC:28:ASP:N	2.53	0.42
8:CC:46:ILE:HD12	35:FI:73:CYS:HB3	2.00	0.42
13:Cg:14:TYR:OH	13:Cg:56:ARG:NH1	2.52	0.42
15:Ck:617:VAL:HG12	15:Ck:618:ILE:HG23	2.02	0.42
16:DB:560:THR:OG1	19:DF:548:ARG:NH1	2.53	0.42
19:DF:196:PHE:HB2	19:DF:227:THR:HG21	2.01	0.42
20:DG:44:ARG:HH11	20:DG:50:LEU:HD13	1.84	0.42
20:DG:351:GLN:HG2	20:DG:355:ARG:HH21	1.85	0.42
27:DX:98:LEU:HD22	27:DX:127:MET:HE3	2.02	0.42
34:FH:414:LYS:HD2	35:FI:72:ARG:HB2	2.01	0.42
10:CJ:315:ASP:OD1	10:CJ:315:ASP:N	2.47	0.42
12:CS:76:THR:OG1	12:CS:138:LYS:NZ	2.47	0.42
15:Ck:688:TYR:HD1	15:Ck:688:TYR:HA	1.76	0.42
16:DB:839:TYR:HE2	16:DB:841:ARG:HH11	1.68	0.42
16:DB:996:ALA:O	16:DB:1000:ARG:HB2	2.20	0.42
17:DC:448:GLU:O	17:DC:452:GLN:NE2	2.47	0.42
29:F1:509:LEU:HB3	29:F1:542:GLN:HE22	1.84	0.42
10:CJ:345:VAL:O	10:CJ:349:THR:OG1	2.31	0.42
19:DF:158:LEU:H	19:DF:163:ARG:HH11	1.66	0.42
24:DT:12:ARG:HH21	34:FH:436:GLN:HE21	1.68	0.42
29:F1:489:MET:HE1	29:F1:507:ARG:HG2	2.01	0.42
47:Uh:1:UNK:N	47:Uh:328:UNK:HG1	2.34	0.42
9:CI:249:GLU:OE2	9:CI:252:ARG:NH2	2.53	0.42
11:CN:28:SER:HA	11:CN:31:MET:HE3	2.02	0.42
15:Ck:572:MET:HE1	15:Ck:575:LEU:HG	2.02	0.42
16:DB:818:GLU:HG3	19:DF:529:PRO:HB3	2.01	0.42
22:DJ:266:VAL:HG21	22:DJ:301:HIS:HD2	1.85	0.42
28:DY:28:GLY:HA3	28:DY:29:PRO:HD3	1.91	0.42
31:FD:245:ASN:OD1	31:FD:245:ASN:N	2.52	0.42
36:FK:94:PRO:HA	36:FK:95:PRO:HD3	1.90	0.42
37:FL:270:LEU:HD21	37:FL:301:LEU:HD11	2.02	0.42
46:Ug:87:UNK:HA	46:Ug:90:UNK:HG3	2.02	0.42
8:CC:74:THR:CG2	37:FL:200:TYR:HD2	2.33	0.42
13:Cg:256:PRO:HG2	15:Ck:830:PHE:HB2	2.02	0.42
19:DF:266:ARG:NH2	19:DF:301:ASN:OD1	2.53	0.42
29:F1:780:ARG:HD2	53:Ux:64:UNK:HA	2.01	0.42
29:F1:798:MET:HA	29:F1:801:VAL:HG12	2.01	0.42
34:FH:112:PRO:O	34:FH:115:SER:OG	2.36	0.42
35:FI:200:ARG:HA	35:FI:204:GLY:HA2	2.02	0.42
13:Cg:294:GLU:OE2	15:Ck:799:LYS:NZ	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:DH:379:LEU:HD23	21:DH:379:LEU:HA	1.95	0.42
29:F1:421:VAL:O	29:F1:425:THR:OG1	2.29	0.42
32:FF:298:LEU:HD21	32:FF:319:LEU:HD12	2.02	0.42
4:FJ:281:SER:HA	29:F1:156:ARG:HH11	1.85	0.41
12:CS:112:THR:HG21	47:Uh:9:UNK:HG2	2.02	0.41
16:DB:1080:ARG:HH21	19:DF:177:ASP:HB2	1.85	0.41
20:DG:160:ARG:NH1	20:DG:163:GLN:OE1	2.43	0.41
21:DH:282:ASN:HD22	21:DH:315:LEU:HD23	1.85	0.41
29:F1:735:LYS:HA	29:F1:735:LYS:HD3	1.91	0.41
31:FD:215:ASP:O	31:FD:219:THR:OG1	2.32	0.41
31:FD:371:ASP:OD1	31:FD:371:ASP:N	2.52	0.41
11:CN:166:ILE:HG21	15:Ck:750:ALA:HA	2.03	0.41
13:Cg:105:HIS:O	13:Cg:107:ARG:NH1	2.53	0.41
15:Ck:686:LYS:HD3	15:Ck:687:ARG:HH21	1.85	0.41
17:DC:619:VAL:HG22	17:DC:767:GLU:HG2	2.01	0.41
18:DE:198:CYS:HA	18:DE:202:HIS:HD2	1.85	0.41
29:F1:732:LYS:HA	29:F1:732:LYS:HD2	1.89	0.41
36:FK:127:PRO:HD2	40:Ua:29:UNK:HG3	2.02	0.41
40:Ua:9:UNK:HA	40:Ua:12:UNK:HG3	2.02	0.41
53:Ux:40:UNK:HA	53:Ux:43:UNK:HG3	2.01	0.41
9:CI:112:GLU:HG3	9:CI:175:ARG:HH12	1.84	0.41
13:Cg:392:LYS:HE2	25:DV:171:ARG:HH22	1.85	0.41
13:Cg:461:GLN:HG2	28:DY:39:VAL:HG21	2.02	0.41
21:DH:208:ASN:OD1	21:DH:244:THR:OG1	2.34	0.41
29:F1:768:PRO:HA	29:F1:888:ASN:HB3	2.01	0.41
30:F4:328:LEU:HD11	30:F4:437:LEU:HD21	2.02	0.41
33:FG:119:LEU:HG	33:FG:123:ILE:HD11	2.01	0.41
13:Cg:148:ASP:OD2	13:Cg:359:ARG:NH2	2.48	0.41
15:Ck:623:LYS:HE2	15:Ck:623:LYS:HB2	1.94	0.41
17:DC:80:LEU:HD11	23:DK:161:LEU:HD23	2.02	0.41
29:F1:485:SER:HA	29:F1:486:PRO:HD3	1.91	0.41
29:F1:622:SER:OG	29:F1:634:LEU:O	2.31	0.41
31:FD:98:ILE:HG23	31:FD:106:ALA:HB1	2.01	0.41
33:FG:36:MET:HE2	33:FG:36:MET:HB3	1.96	0.41
7:CA:393:U:H2'	7:CA:394:A:H8	1.85	0.41
7:CA:487:A:H5''	29:F1:830:GLY:HA3	2.01	0.41
8:CC:27:ILE:HA	35:FI:201:MET:HG2	2.02	0.41
9:CI:136:GLN:HG3	9:CI:140:GLU:HB3	2.01	0.41
13:Cg:43:ARG:HH21	13:Cg:52:ARG:HE	1.67	0.41
15:Ck:307:MET:HE1	16:DB:893:ILE:HD11	2.00	0.41
18:DE:587:MET:HE3	18:DE:587:MET:HB2	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:DG:396:ASN:HD21	20:DG:398:ILE:HD12	1.85	0.41
21:DH:85:LEU:O	21:DH:90:ARG:NH2	2.54	0.41
31:FD:130:LEU:HG	35:FI:93:ARG:HG2	2.02	0.41
35:FI:228:GLN:HE22	35:FI:323:LEU:HD13	1.84	0.41
48:Ui:19:UNK:O	48:Ui:22:UNK:HG3	2.21	0.41
10:CJ:143:TYR:OH	25:DV:130:PRO:O	2.31	0.41
15:Ck:668:PHE:HZ	15:Ck:716:ARG:HB2	1.84	0.41
15:Ck:832:THR:HB	15:Ck:835:GLU:HG3	2.02	0.41
17:DC:272:GLU:HA	17:DC:275:LYS:HE3	2.03	0.41
18:DE:331:LYS:HB2	18:DE:336:ILE:HD11	2.02	0.41
33:FG:46:GLY:H	33:FG:49:ASN:HB2	1.86	0.41
10:CJ:551:ARG:NH1	10:CJ:589:GLU:O	2.54	0.41
13:Cg:383:ASP:OD2	25:DV:96:ARG:NH2	2.54	0.41
15:Ck:316:ASP:OD1	15:Ck:316:ASP:N	2.54	0.41
17:DC:888:LEU:HD23	17:DC:888:LEU:HA	1.91	0.41
20:DG:71:ASN:HD22	20:DG:71:ASN:HA	1.66	0.41
24:DT:191:PRO:HB2	24:DT:206:LEU:HD21	2.03	0.41
32:FF:349:ARG:HD3	32:FF:349:ARG:HA	1.93	0.41
10:CJ:105:ASN:ND2	21:DH:491:ASP:OD2	2.45	0.41
10:CJ:293:ASP:OD1	21:DH:311:ARG:NH2	2.52	0.41
10:CJ:719:PRO:HG2	13:Cg:321:TYR:CZ	2.56	0.41
15:Ck:711:ILE:HG21	15:Ck:730:GLU:HG3	2.03	0.41
16:DB:535:THR:HG23	16:DB:538:ARG:HH21	1.86	0.41
19:DF:314:TYR:O	19:DF:318:MET:HB2	2.21	0.41
20:DG:177:GLU:OE2	20:DG:213:ARG:NE	2.54	0.41
24:DT:11:ASP:HB3	38:FV:212:THR:HG23	2.02	0.41
28:DY:53:LEU:HD23	28:DY:53:LEU:HA	1.90	0.41
29:F1:391:LYS:HD3	32:FF:117:LEU:HD22	2.02	0.41
29:F1:669:MET:HE2	29:F1:669:MET:HB2	1.98	0.41
37:FL:10:SER:OG	37:FL:11:TYR:N	2.54	0.41
13:Cg:96:ARG:O	54:CgA:1:GTP:O3'	2.35	0.41
14:Ci:114:MET:HG2	15:Ck:690:TRP:CZ3	2.55	0.41
15:Ck:367:LEU:HD12	15:Ck:578:ALA:HB1	2.03	0.41
16:DB:1019:ALA:HA	16:DB:1038:TYR:HE1	1.86	0.41
16:DB:1066:ASN:OD1	16:DB:1066:ASN:N	2.53	0.41
16:DB:1101:GLN:OE1	19:DF:224:ARG:NH2	2.52	0.41
17:DC:940:ALA:HA	17:DC:944:GLU:HB2	2.03	0.41
20:DG:199:LEU:HD23	20:DG:199:LEU:HA	1.89	0.41
29:F1:690:ASP:OD2	40:Ua:21:UNK:HG1	2.20	0.41
30:F4:208:GLY:HA2	30:F4:227:LEU:O	2.20	0.41
35:FI:122:GLN:HB2	35:FI:140:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:Fe:42:ASN:O	39:Fe:47:ARG:NH2	2.53	0.41
53:Ux:14:UNK:HG2	53:Ux:50:UNK:O	2.21	0.41
7:CA:444:A:OP1	29:F1:833:GLN:NE2	2.44	0.41
8:CC:74:THR:OG1	37:FL:200:TYR:CD2	2.72	0.41
9:CI:126:TRP:CG	9:CI:148:LEU:HD11	2.56	0.41
24:DT:32:TRP:HA	24:DT:219:GLN:O	2.21	0.41
29:F1:315:TYR:HB3	29:F1:318:LEU:HD23	2.02	0.41
30:F4:460:ASP:OD2	30:F4:460:ASP:N	2.52	0.41
36:FK:245:GLU:O	36:FK:261:VAL:N	2.50	0.41
46:Ug:115:UNK:HA	46:Ug:118:UNK:HG3	2.03	0.41
6:Fa:133:LEU:HD11	9:CI:229:HIS:HD2	1.86	0.40
7:CA:515:U:H2'	32:FF:434:ALA:HB1	2.03	0.40
10:CJ:368:VAL:HG12	10:CJ:395:ARG:HB3	2.04	0.40
13:Cg:138:LEU:HD22	25:DV:179:LEU:HD13	2.03	0.40
17:DC:192:SER:O	17:DC:197:LYS:N	2.54	0.40
29:F1:457:LEU:HD22	29:F1:803:GLN:HE22	1.85	0.40
35:FI:222:ALA:HA	35:FI:225:LYS:HE2	2.03	0.40
37:FL:49:LYS:NZ	37:FL:50:GLY:O	2.52	0.40
6:Fa:134:PRO:HB3	9:CI:190:GLN:HB2	2.03	0.40
9:CI:316:LYS:HB2	9:CI:316:LYS:HE3	1.90	0.40
10:CJ:555:TRP:HB2	10:CJ:582:LYS:HD3	2.02	0.40
11:CN:51:LEU:HD23	11:CN:55:LEU:HD23	2.04	0.40
15:Ck:150:VAL:HG11	15:Ck:247:LEU:HD22	2.03	0.40
16:DB:546:ARG:HH11	16:DB:877:PRO:HD3	1.85	0.40
16:DB:990:ARG:HA	16:DB:990:ARG:HD2	1.84	0.40
17:DC:953:MET:HE2	17:DC:953:MET:HB3	1.93	0.40
18:DE:49:MET:HE1	18:DE:91:GLY:HA2	2.03	0.40
19:DF:443:LEU:HD13	19:DF:452:VAL:HG11	2.03	0.40
20:DG:325:TYR:O	20:DG:373:TRP:NE1	2.52	0.40
20:DG:626:LEU:HD23	20:DG:626:LEU:HA	1.92	0.40
22:DJ:122:ALA:O	22:DJ:164:SER:OG	2.36	0.40
23:DK:242:HIS:HD2	23:DK:243:PRO:HD2	1.85	0.40
24:DT:35:LYS:HB2	24:DT:35:LYS:HE3	1.91	0.40
35:FI:142:ASN:OD1	35:FI:142:ASN:N	2.52	0.40
36:FK:103:LEU:HD23	36:FK:370:VAL:HG11	2.03	0.40
46:Ug:78:UNK:O	46:Ug:82:UNK:HG3	2.20	0.40
47:Uh:298:UNK:HG2	47:Uh:311:UNK:HB1	2.02	0.40
8:CC:74:THR:CG2	37:FL:200:TYR:HA	2.49	0.40
9:CI:329:HIS:ND1	9:CI:367:ASP:OD1	2.51	0.40
10:CJ:230:PHE:O	10:CJ:239:ARG:NH1	2.54	0.40
13:Cg:233:THR:OG1	13:Cg:239:GLN:NE2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:Ci:33:LEU:HD13	15:Ck:735:ILE:HG21	2.04	0.40
15:Ck:366:PHE:HB3	15:Ck:582:THR:HG21	2.03	0.40
26:DW:70:LEU:HD11	28:DY:48:LEU:HD21	2.04	0.40
30:F4:353:LEU:HD21	40:Ua:41:UNK:HG1	2.03	0.40
31:FD:401:VAL:HG11	48:Ui:8:UNK:HG2	2.02	0.40
39:Fe:54:ARG:HG2	39:Fe:69:ILE:HG22	2.03	0.40
7:CA:449:G:OP1	21:DH:538:ARG:NH1	2.49	0.40
11:CN:40:TRP:HD1	14:Ci:93:LEU:HD11	1.86	0.40
15:Ck:119:GLU:OE1	15:Ck:132:TYR:OH	2.34	0.40
17:DC:157:ASN:HB3	31:FD:315:ARG:HB2	2.03	0.40
17:DC:316:THR:HB	17:DC:319:GLU:HG3	2.04	0.40
18:DE:296:LEU:HA	18:DE:299:LYS:HG2	2.04	0.40
24:DT:135:ILE:HG12	24:DT:160:TYR:HB2	2.03	0.40
29:F1:165:ARG:NH1	29:F1:529:GLU:OE1	2.54	0.40
30:F4:485:LEU:HD23	30:F4:485:LEU:HA	1.94	0.40
37:FL:12:THR:HA	37:FL:13:PRO:HD3	1.94	0.40
37:FL:172:VAL:HG13	37:FL:192:LEU:HD12	2.03	0.40
4:FJ:278:GLU:OE2	32:FF:427:ARG:NH2	2.55	0.40
10:CJ:304:ARG:HE	15:Ck:665:PRO:HG3	1.86	0.40
10:CJ:489:TRP:HE1	10:CJ:512:THR:HA	1.86	0.40
12:CS:93:ASP:OD2	12:CS:93:ASP:N	2.54	0.40
13:Cg:390:PRO:O	13:Cg:394:SER:OG	2.30	0.40
18:DE:182:ASP:HB3	18:DE:190:PHE:HE2	1.86	0.40
18:DE:407:MET:HE3	18:DE:407:MET:HB3	1.74	0.40
20:DG:497:ARG:HD2	20:DG:497:ARG:HA	1.93	0.40
30:F4:65:ASP:N	30:F4:65:ASP:OD1	2.53	0.40
30:F4:482:LEU:HD11	30:F4:568:THR:HG22	2.04	0.40
33:FG:116:ARG:NH2	38:FV:128:LEU:O	2.55	0.40
34:FH:317:GLU:HG3	34:FH:391:LEU:HD13	2.03	0.40
48:Ui:5:UNK:HA	48:Ui:8:UNK:HG3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CE	21/435 (5%)	21 (100%)	0	0	100	100
2	CK	38/326 (12%)	36 (95%)	2 (5%)	0	100	100
3	Cn	16/250 (6%)	14 (88%)	2 (12%)	0	100	100
4	FJ	39/362 (11%)	39 (100%)	0	0	100	100
5	FY	90/188 (48%)	85 (94%)	5 (6%)	0	100	100
6	Fa	37/171 (22%)	35 (95%)	2 (5%)	0	100	100
8	CC	72/74 (97%)	72 (100%)	0	0	100	100
9	CI	421/443 (95%)	405 (96%)	16 (4%)	0	100	100
10	CJ	695/817 (85%)	655 (94%)	36 (5%)	4 (1%)	21	52
11	CN	151/166 (91%)	149 (99%)	2 (1%)	0	100	100
12	CS	79/244 (32%)	74 (94%)	5 (6%)	0	100	100
13	Cg	482/498 (97%)	463 (96%)	19 (4%)	0	100	100
14	Ci	145/181 (80%)	138 (95%)	7 (5%)	0	100	100
15	Ck	634/874 (72%)	600 (95%)	34 (5%)	0	100	100
16	DB	671/1181 (57%)	648 (97%)	23 (3%)	0	100	100
17	DC	1020/1165 (88%)	998 (98%)	22 (2%)	0	100	100
18	DE	582/747 (78%)	564 (97%)	16 (3%)	2 (0%)	36	67
19	DF	485/666 (73%)	466 (96%)	19 (4%)	0	100	100
20	DG	558/631 (88%)	545 (98%)	13 (2%)	0	100	100
21	DH	466/581 (80%)	445 (96%)	21 (4%)	0	100	100
22	DJ	304/396 (77%)	296 (97%)	8 (3%)	0	100	100
23	DK	239/324 (74%)	228 (95%)	11 (5%)	0	100	100
24	DT	219/247 (89%)	208 (95%)	11 (5%)	0	100	100
25	DV	153/183 (84%)	147 (96%)	6 (4%)	0	100	100
26	DW	131/179 (73%)	121 (92%)	10 (8%)	0	100	100
27	DX	113/169 (67%)	109 (96%)	4 (4%)	0	100	100
28	DY	152/163 (93%)	147 (97%)	5 (3%)	0	100	100
29	F1	827/1041 (79%)	792 (96%)	35 (4%)	0	100	100
30	F4	521/811 (64%)	490 (94%)	30 (6%)	1 (0%)	43	73
31	FD	392/579 (68%)	386 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	FF	404/474 (85%)	389 (96%)	13 (3%)	2 (0%)	24	57
33	FG	167/463 (36%)	162 (97%)	5 (3%)	0	100	100
34	FH	313/457 (68%)	303 (97%)	10 (3%)	0	100	100
35	FI	342/445 (77%)	333 (97%)	9 (3%)	0	100	100
36	FK	202/372 (54%)	200 (99%)	2 (1%)	0	100	100
37	FL	314/353 (89%)	298 (95%)	16 (5%)	0	100	100
38	FV	206/264 (78%)	199 (97%)	7 (3%)	0	100	100
39	Fe	120/123 (98%)	113 (94%)	7 (6%)	0	100	100
All	All	11821/17043 (69%)	11373 (96%)	439 (4%)	9 (0%)	49	78

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	DE	521	PRO
10	CJ	592	SER
10	CJ	238	ILE
30	F4	590	ASN
10	CJ	236	ASP
10	CJ	237	GLY
32	FF	125	LEU
32	FF	126	VAL
18	DE	476	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CE	22/372 (6%)	22 (100%)	0	100	100
2	CK	37/284 (13%)	37 (100%)	0	100	100
3	Cn	14/210 (7%)	14 (100%)	0	100	100
4	FJ	38/323 (12%)	38 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	FY	77/163 (47%)	77 (100%)	0	100	100
6	Fa	30/149 (20%)	30 (100%)	0	100	100
8	CC	73/73 (100%)	71 (97%)	2 (3%)	39	67
9	CI	355/371 (96%)	354 (100%)	1 (0%)	86	87
10	CJ	619/723 (86%)	617 (100%)	2 (0%)	86	87
11	CN	138/150 (92%)	138 (100%)	0	100	100
12	CS	76/220 (34%)	76 (100%)	0	100	100
13	Cg	426/437 (98%)	424 (100%)	2 (0%)	81	85
14	Ci	130/160 (81%)	129 (99%)	1 (1%)	73	81
15	Ck	557/747 (75%)	555 (100%)	2 (0%)	84	86
16	DB	613/1030 (60%)	612 (100%)	1 (0%)	87	89
17	DC	867/985 (88%)	866 (100%)	1 (0%)	88	90
18	DE	464/644 (72%)	464 (100%)	0	100	100
19	DF	417/560 (74%)	417 (100%)	0	100	100
20	DG	490/543 (90%)	489 (100%)	1 (0%)	87	89
21	DH	413/504 (82%)	412 (100%)	1 (0%)	87	89
22	DJ	267/347 (77%)	267 (100%)	0	100	100
23	DK	203/261 (78%)	203 (100%)	0	100	100
24	DT	205/228 (90%)	205 (100%)	0	100	100
25	DV	142/165 (86%)	142 (100%)	0	100	100
26	DW	124/163 (76%)	123 (99%)	1 (1%)	73	81
27	DX	102/149 (68%)	101 (99%)	1 (1%)	68	79
28	DY	137/146 (94%)	136 (99%)	1 (1%)	76	82
29	F1	718/895 (80%)	718 (100%)	0	100	100
30	F4	479/703 (68%)	476 (99%)	3 (1%)	78	83
31	FD	338/494 (68%)	338 (100%)	0	100	100
32	FF	348/400 (87%)	346 (99%)	2 (1%)	78	83
33	FG	147/414 (36%)	147 (100%)	0	100	100
34	FH	270/390 (69%)	269 (100%)	1 (0%)	84	86
35	FI	297/380 (78%)	297 (100%)	0	100	100
36	FK	181/308 (59%)	181 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	FL	279/309 (90%)	279 (100%)	0	100	100
38	FV	184/231 (80%)	184 (100%)	0	100	100
39	Fe	114/115 (99%)	114 (100%)	0	100	100
All	All	10391/14746 (70%)	10368 (100%)	23 (0%)	85	89

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	CC	28	ASP
8	CC	74	THR
9	CI	281	VAL
10	CJ	375	THR
10	CJ	803	ILE
13	Cg	54	VAL
13	Cg	260	ASP
14	Ci	114	MET
15	Ck	172	ILE
15	Ck	573	THR
16	DB	744	VAL
17	DC	150	LEU
20	DG	466	VAL
21	DH	107	THR
26	DW	169	VAL
27	DX	149	THR
28	DY	136	VAL
30	F4	459	VAL
30	F4	523	VAL
30	F4	807	LEU
32	FF	134	THR
32	FF	415	THR
34	FH	252	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (226) such sidechains are listed below:

Mol	Chain	Res	Type
2	CK	56	GLN
5	FY	35	ASN
5	FY	104	GLN
8	CC	31	ASN
8	CC	48	HIS

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Mol	Chain	Res	Type
9	CI	77	ASN
9	CI	79	GLN
9	CI	84	ASN
9	CI	136	GLN
9	CI	208	HIS
9	CI	229	HIS
9	CI	397	ASN
10	CJ	151	ASN
10	CJ	170	HIS
10	CJ	172	GLN
10	CJ	360	HIS
10	CJ	426	GLN
10	CJ	432	HIS
10	CJ	450	HIS
10	CJ	460	HIS
10	CJ	476	ASN
10	CJ	632	GLN
10	CJ	670	GLN
10	CJ	728	GLN
10	CJ	761	GLN
10	CJ	776	GLN
10	CJ	791	HIS
10	CJ	798	GLN
10	CJ	804	ASN
11	CN	42	HIS
11	CN	63	HIS
11	CN	96	HIS
11	CN	112	ASN
11	CN	153	ASN
12	CS	88	ASN
13	Cg	75	ASN
13	Cg	87	GLN
13	Cg	99	GLN
13	Cg	241	GLN
13	Cg	242	ASN
13	Cg	397	HIS
13	Cg	453	GLN
13	Cg	460	HIS
13	Cg	474	GLN
14	Ci	82	GLN
14	Ci	125	HIS
15	Ck	97	GLN

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Mol	Chain	Res	Type
15	Ck	113	ASN
15	Ck	134	HIS
15	Ck	195	GLN
15	Ck	215	HIS
15	Ck	285	ASN
15	Ck	361	GLN
15	Ck	399	ASN
15	Ck	417	ASN
15	Ck	543	GLN
15	Ck	589	GLN
15	Ck	611	ASN
15	Ck	644	HIS
15	Ck	679	GLN
15	Ck	695	GLN
15	Ck	728	GLN
16	DB	542	GLN
16	DB	684	GLN
16	DB	703	HIS
16	DB	707	GLN
16	DB	737	HIS
16	DB	800	GLN
16	DB	958	ASN
16	DB	1051	GLN
16	DB	1064	GLN
17	DC	81	HIS
17	DC	157	ASN
17	DC	227	GLN
17	DC	263	GLN
17	DC	303	HIS
17	DC	368	ASN
17	DC	375	HIS
17	DC	473	GLN
17	DC	500	ASN
17	DC	520	ASN
17	DC	548	HIS
17	DC	682	ASN
17	DC	691	GLN
17	DC	776	ASN
17	DC	797	ASN
17	DC	841	HIS
17	DC	871	GLN
17	DC	951	ASN

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Mol	Chain	Res	Type
18	DE	84	HIS
18	DE	189	HIS
18	DE	202	HIS
18	DE	319	ASN
18	DE	345	ASN
18	DE	442	HIS
18	DE	534	ASN
18	DE	596	HIS
18	DE	650	HIS
18	DE	658	ASN
18	DE	699	ASN
18	DE	703	GLN
19	DF	128	HIS
19	DF	175	GLN
19	DF	178	ASN
19	DF	187	ASN
19	DF	283	HIS
19	DF	376	ASN
19	DF	396	GLN
19	DF	404	GLN
19	DF	520	GLN
19	DF	542	HIS
19	DF	556	HIS
19	DF	572	HIS
19	DF	592	HIS
20	DG	23	HIS
20	DG	26	ASN
20	DG	71	ASN
20	DG	92	GLN
20	DG	143	HIS
20	DG	170	ASN
20	DG	191	GLN
20	DG	200	GLN
20	DG	201	GLN
20	DG	229	HIS
20	DG	230	ASN
20	DG	351	GLN
20	DG	476	GLN
20	DG	477	GLN
21	DH	123	HIS
21	DH	160	ASN
21	DH	191	HIS

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Mol	Chain	Res	Type
21	DH	257	ASN
21	DH	275	HIS
21	DH	327	HIS
21	DH	343	ASN
21	DH	356	GLN
22	DJ	33	ASN
22	DJ	42	HIS
22	DJ	56	HIS
22	DJ	174	ASN
22	DJ	190	ASN
22	DJ	199	GLN
23	DK	132	HIS
23	DK	163	HIS
23	DK	171	GLN
23	DK	242	HIS
24	DT	72	HIS
24	DT	113	GLN
24	DT	140	ASN
24	DT	192	GLN
24	DT	219	GLN
25	DV	38	GLN
25	DV	40	HIS
25	DV	51	ASN
25	DV	145	ASN
25	DV	170	GLN
26	DW	44	ASN
26	DW	66	HIS
26	DW	69	GLN
26	DW	120	ASN
26	DW	154	HIS
27	DX	58	HIS
28	DY	41	GLN
28	DY	99	GLN
28	DY	106	GLN
29	F1	331	HIS
29	F1	332	GLN
29	F1	344	GLN
29	F1	477	GLN
29	F1	502	ASN
29	F1	517	GLN
29	F1	542	GLN
29	F1	563	ASN

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Mol	Chain	Res	Type
29	F1	763	ASN
29	F1	776	HIS
29	F1	803	GLN
29	F1	810	GLN
30	F4	56	GLN
30	F4	126	HIS
30	F4	266	ASN
30	F4	334	GLN
30	F4	348	ASN
30	F4	479	ASN
30	F4	483	GLN
30	F4	686	HIS
30	F4	800	ASN
31	FD	46	HIS
31	FD	100	HIS
31	FD	240	GLN
31	FD	241	HIS
31	FD	269	ASN
31	FD	272	HIS
31	FD	346	GLN
32	FF	438	HIS
32	FF	443	ASN
33	FG	64	HIS
33	FG	69	GLN
33	FG	145	ASN
34	FH	111	HIS
34	FH	134	ASN
34	FH	315	ASN
34	FH	436	GLN
34	FH	451	ASN
35	FI	50	GLN
35	FI	97	HIS
35	FI	120	GLN
35	FI	153	GLN
35	FI	219	ASN
35	FI	228	GLN
35	FI	322	ASN
36	FK	169	GLN
36	FK	263	HIS
36	FK	312	ASN
37	FL	23	ASN
37	FL	69	ASN

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Mol	Chain	Res	Type
37	FL	70	ASN
37	FL	224	ASN
37	FL	263	HIS
37	FL	335	GLN
37	FL	349	ASN
38	FV	76	GLN
38	FV	194	HIS
39	Fe	22	ASN
39	Fe	42	ASN
39	Fe	101	GLN
39	Fe	117	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
7	CA	145/802 (18%)	55 (37%)	1 (0%)

All (55) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	CA	388	U
7	CA	389	A
7	CA	390	U
7	CA	396	A
7	CA	397	U
7	CA	398	U
7	CA	399	A
7	CA	400	U
7	CA	405	A
7	CA	413	A
7	CA	416	U
7	CA	417	A
7	CA	418	A
7	CA	421	G
7	CA	422	G
7	CA	425	A
7	CA	429	U
7	CA	430	U
7	CA	431	U
7	CA	432	G
7	CA	433	U

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Mol	Chain	Res	Type
7	CA	435	G
7	CA	438	U
7	CA	439	U
7	CA	443	U
7	CA	444	A
7	CA	445	C
7	CA	446	C
7	CA	447	A
7	CA	448	U
7	CA	454	G
7	CA	455	G
7	CA	459	A
7	CA	460	U
7	CA	461	A
7	CA	470	G
7	CA	471	U
7	CA	473	U
7	CA	480	C
7	CA	481	A
7	CA	484	A
7	CA	489	A
7	CA	490	A
7	CA	498	U
7	CA	503	A
7	CA	509	U
7	CA	513	U
7	CA	515	U
7	CA	516	G
7	CA	520	A
7	CA	524	A
7	CA	525	A
7	CA	527	A
7	CA	528	U
7	CA	529	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	CA	483	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 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$
57	SAH	F1B	1	-	27,28,28	1.08	4 (14%)	36,40,40	2.07	10 (27%)
54	GTP	CgA	1	-	33,34,34	0.91	0	50,54,54	1.72	9 (18%)
57	SAH	FFA	1	-	27,28,28	1.11	4 (14%)	36,40,40	2.09	10 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	SAH	F1B	1	-	-	4/15/31/31	0/3/3/3
54	GTP	CgA	1	-	-	5/22/38/38	0/3/3/3
57	SAH	FFA	1	-	-	1/15/31/31	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	FFA	1	SAH	C2-N3	2.59	1.38	1.33
57	FFA	1	SAH	C2-N1	2.55	1.38	1.33
57	F1B	1	SAH	C2-N1	2.48	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	F1B	1	SAH	C2-N3	2.45	1.38	1.33
57	F1B	1	SAH	OXT-C	-2.25	1.23	1.30
57	FFA	1	SAH	OXT-C	-2.25	1.23	1.30
57	FFA	1	SAH	C5-N7	-2.12	1.35	1.39
57	F1B	1	SAH	C8-N7	2.05	1.35	1.31

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	CgA	1	GTP	C5-C4-N3	-5.82	119.12	128.39
57	F1B	1	SAH	N3-C2-N1	-5.53	120.21	128.58
57	FFA	1	SAH	N3-C2-N1	-5.47	120.30	128.58
54	CgA	1	GTP	C2-N3-C4	5.22	121.30	112.30
57	FFA	1	SAH	C5-C4-N3	-4.84	120.05	126.72
57	F1B	1	SAH	C5-C4-N3	-4.57	120.42	126.72
57	FFA	1	SAH	C5'-SD-CG	-4.25	89.64	102.26
57	F1B	1	SAH	C5'-SD-CG	-3.98	90.45	102.26
57	F1B	1	SAH	N9-C8-N7	-3.79	108.56	113.94
54	CgA	1	GTP	N9-C4-N3	3.79	133.52	125.95
57	FFA	1	SAH	N9-C8-N7	-3.65	108.75	113.94
57	FFA	1	SAH	C2-N3-C4	3.49	120.35	111.83
57	F1B	1	SAH	C2-N3-C4	3.47	120.31	111.83
57	FFA	1	SAH	N3-C4-N9	3.36	132.89	127.17
57	F1B	1	SAH	C5-N7-C8	3.33	108.69	103.45
57	FFA	1	SAH	C5-N7-C8	3.29	108.62	103.45
54	CgA	1	GTP	C2-N1-C6	-3.13	119.44	125.11
57	F1B	1	SAH	N3-C4-N9	2.96	132.20	127.17
54	CgA	1	GTP	C3'-C2'-C1'	2.67	106.50	101.46
57	FFA	1	SAH	OXT-C-O	-2.65	118.07	124.08
57	F1B	1	SAH	OXT-C-O	-2.64	118.09	124.08
54	CgA	1	GTP	C5-C6-N1	2.58	119.83	113.25
54	CgA	1	GTP	O6-C6-C5	-2.43	120.12	126.53
54	CgA	1	GTP	C8-N7-C5	2.42	108.57	104.26
57	F1B	1	SAH	C4-C5-N7	-2.36	107.88	110.58
57	F1B	1	SAH	O4'-C1'-N9	2.29	112.49	108.09
54	CgA	1	GTP	N9-C8-N7	-2.24	109.24	113.40
57	FFA	1	SAH	C4-C5-N7	-2.18	108.09	110.58
57	FFA	1	SAH	C6-C5-C4	2.01	119.92	117.18

There are no chirality outliers.

All (10) torsion outliers are listed below:

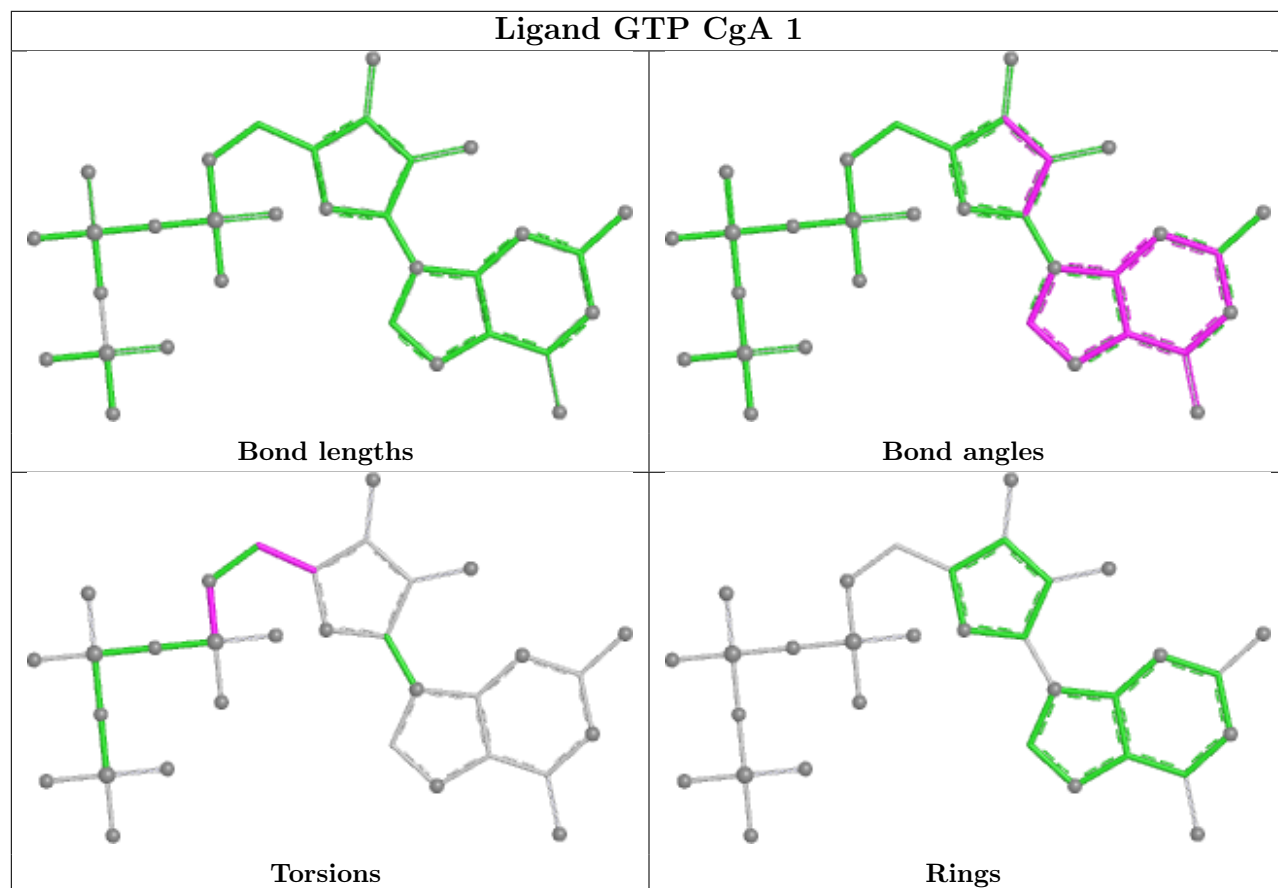
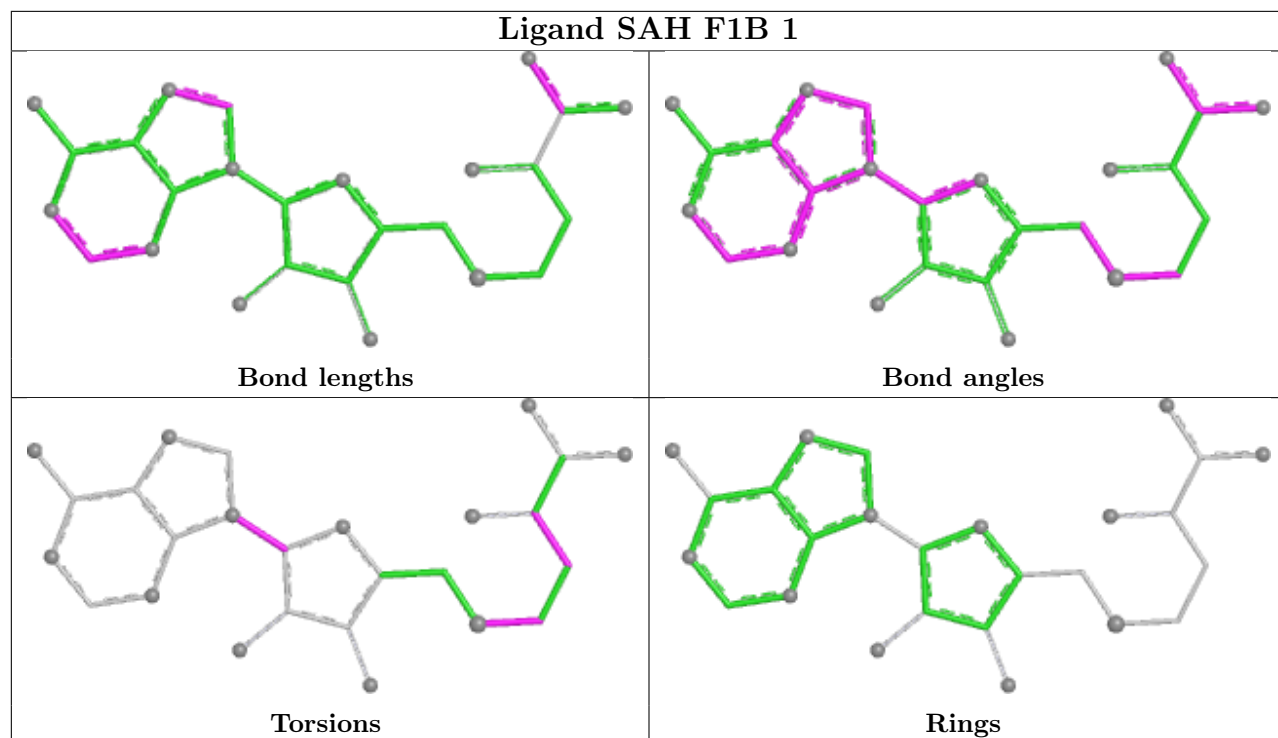
Mol	Chain	Res	Type	Atoms
54	CgA	1	GTP	C5'-O5'-PA-O3A
54	CgA	1	GTP	C5'-O5'-PA-O1A
54	CgA	1	GTP	C5'-O5'-PA-O2A
57	F1B	1	SAH	N-CA-CB-CG
57	F1B	1	SAH	C-CA-CB-CG
54	CgA	1	GTP	C3'-C4'-C5'-O5'
54	CgA	1	GTP	O4'-C4'-C5'-O5'
57	F1B	1	SAH	CB-CG-SD-C5'
57	FFA	1	SAH	C3'-C4'-C5'-SD
57	F1B	1	SAH	C2'-C1'-N9-C8

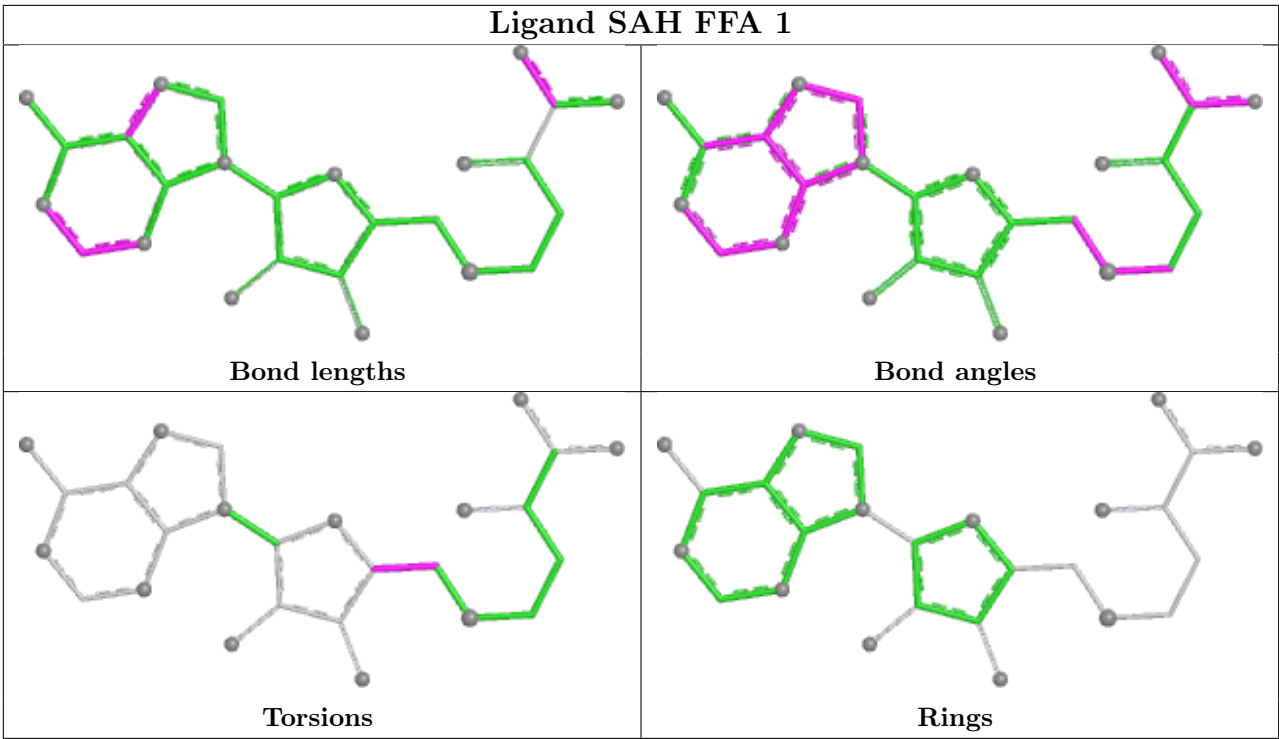
There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	F1B	1	SAH	2	0
54	CgA	1	GTP	4	0
57	FFA	1	SAH	4	0

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





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
47	Uh	11
46	Ug	10
53	Ux	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Uh	219:UNK	C	267:UNK	N	51.70
1	Uh	13:UNK	C	14:UNK	N	49.42
1	Uh	88:UNK	C	98:UNK	N	42.41
1	Uh	124:UNK	C	125:UNK	N	39.54
1	Uh	199:UNK	C	200:UNK	N	38.31
1	Ug	129:UNK	C	130:UNK	N	35.86
1	Uh	145:UNK	C	184:UNK	N	35.70
1	Ug	102:UNK	C	103:UNK	N	29.52

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Uh	39:UNK	C	40:UNK	N	25.40
1	Ug	83:UNK	C	84:UNK	N	24.22
1	Uh	68:UNK	C	69:UNK	N	21.45
1	Uh	134:UNK	C	135:UNK	N	17.15
1	Uh	280:UNK	C	281:UNK	N	15.55
1	Ux	15:UNK	C	28:UNK	N	14.78
1	Ux	66:UNK	C	74:UNK	N	12.83
1	Ug	52:UNK	C	53:UNK	N	12.79
1	Ug	70:UNK	C	71:UNK	N	12.48
1	Ux	47:UNK	C	49:UNK	N	12.00
1	Ug	39:UNK	C	40:UNK	N	10.97
1	Ug	26:UNK	C	27:UNK	N	8.39
1	Uh	323:UNK	C	324:UNK	N	7.01
1	Ug	46:UNK	C	47:UNK	N	6.52
1	Ug	145:UNK	C	146:UNK	N	4.54
1	Ug	33:UNK	C	34:UNK	N	4.41

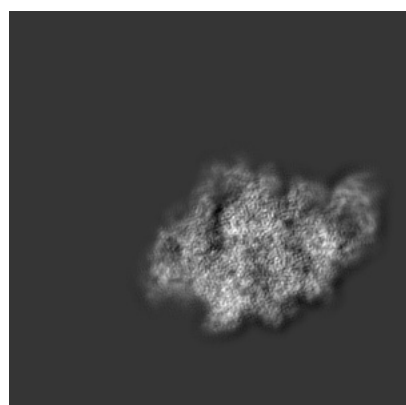
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10175. These allow visual inspection of the internal detail of the map and identification of artifacts.

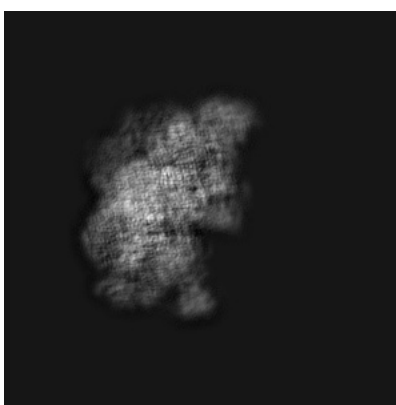
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

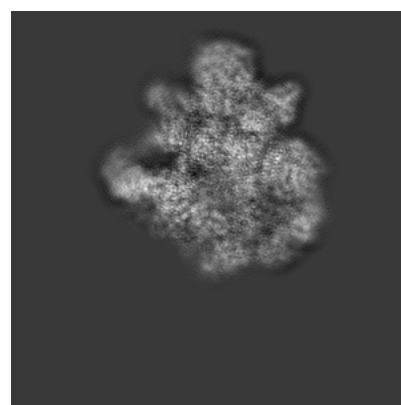
6.1.1 Primary map



X



Y

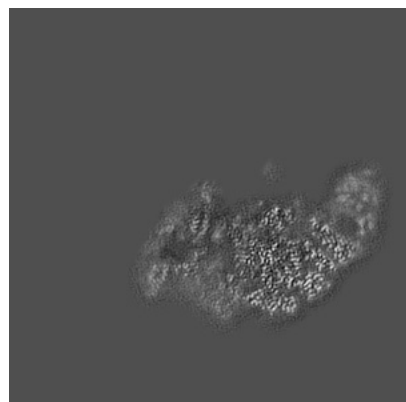


Z

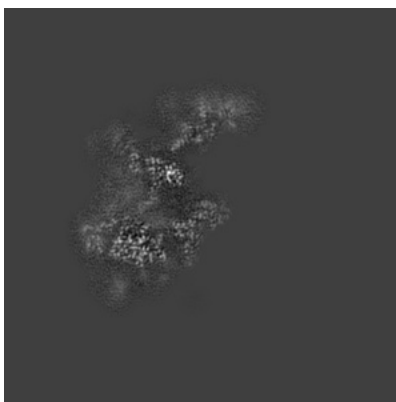
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

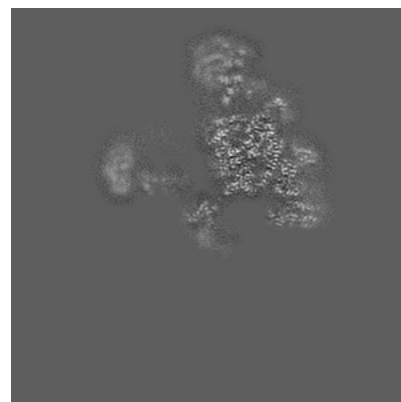
6.2.1 Primary map



X Index: 160



Y Index: 160

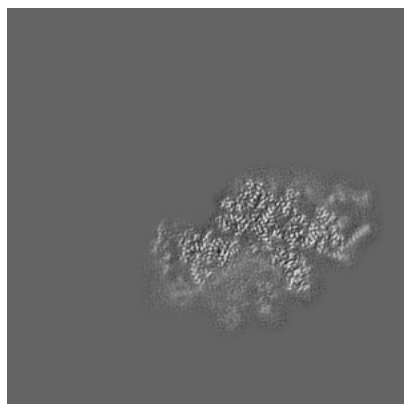


Z Index: 160

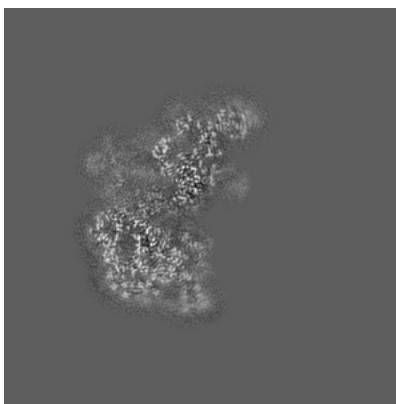
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

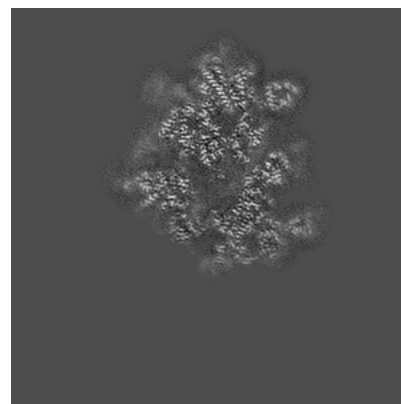
6.3.1 Primary map



X Index: 190



Y Index: 183

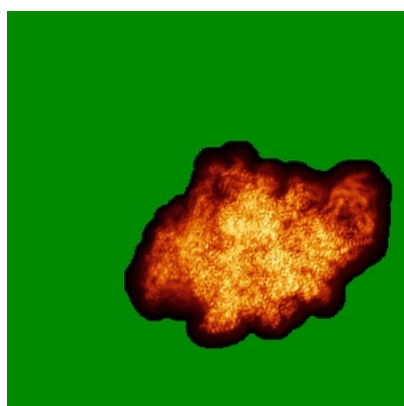


Z Index: 126

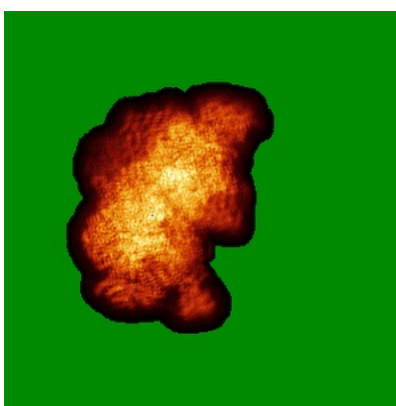
The images above show the largest variance slices of the map in three orthogonal directions.

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

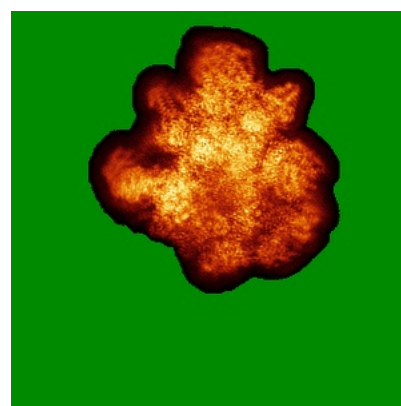
6.4.1 Primary map



X



Y

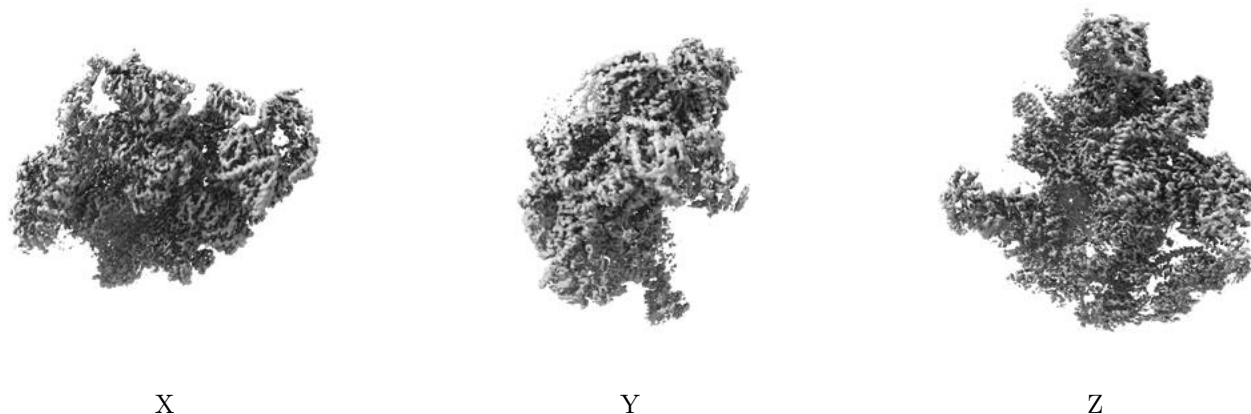


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0793. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

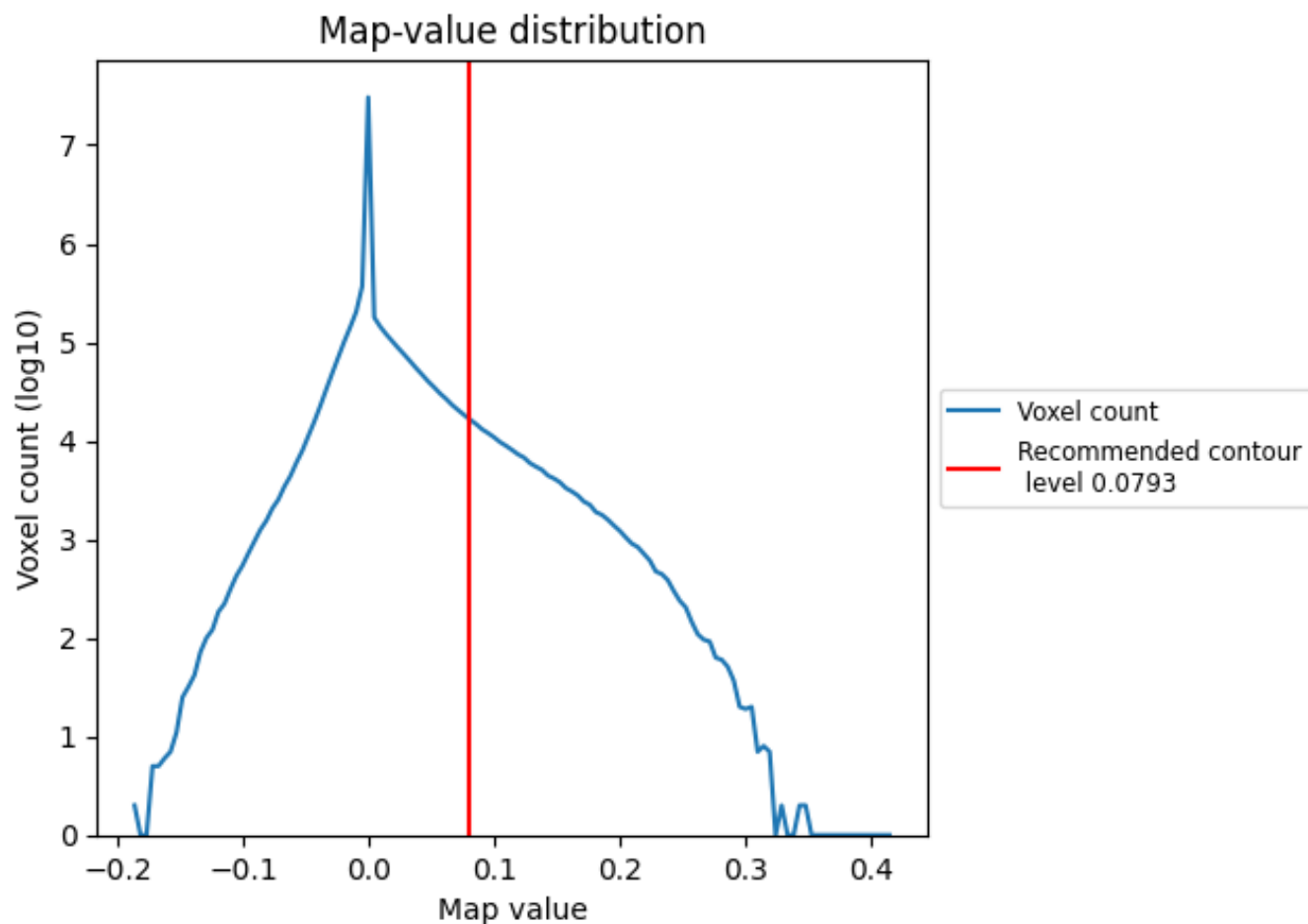
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

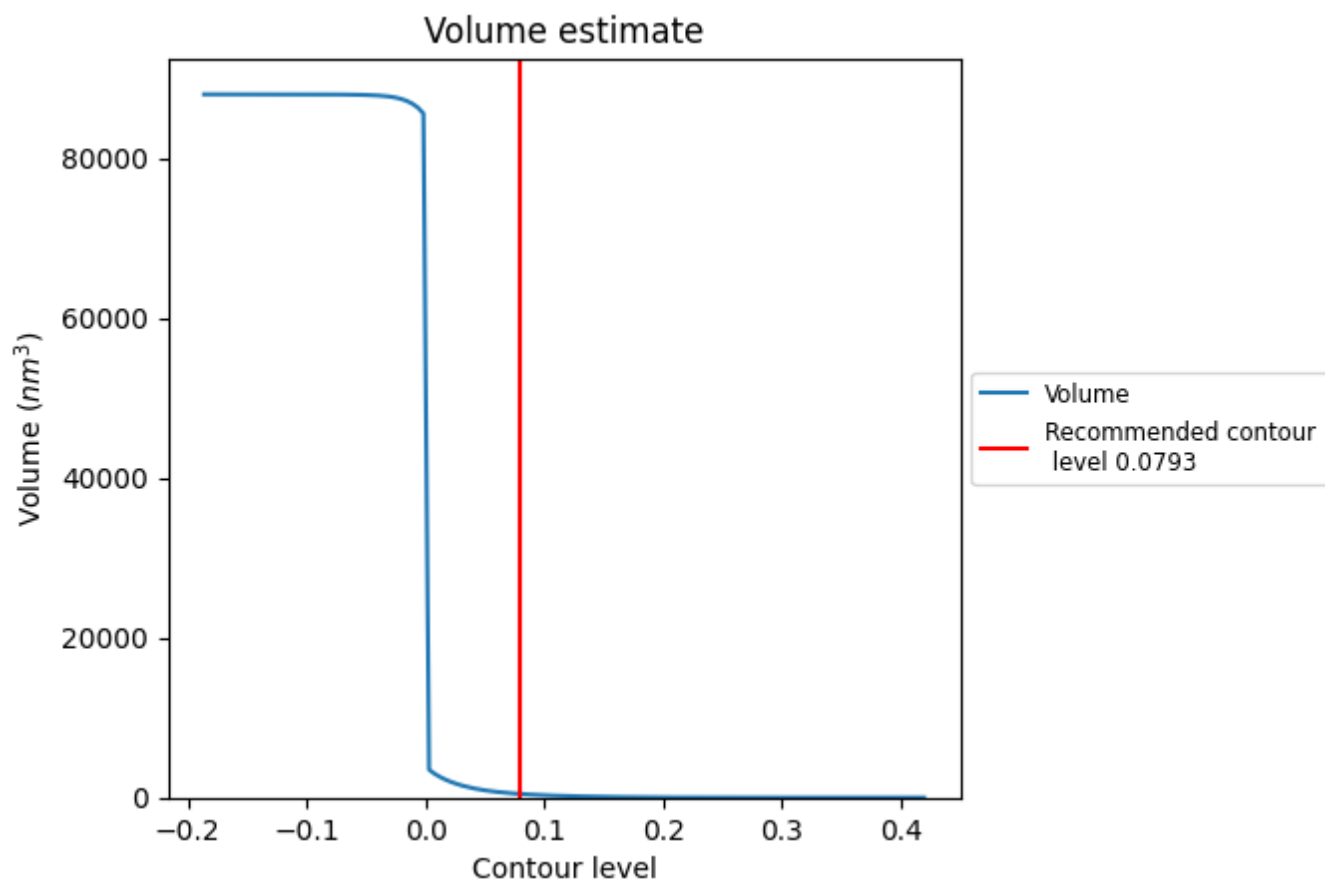
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

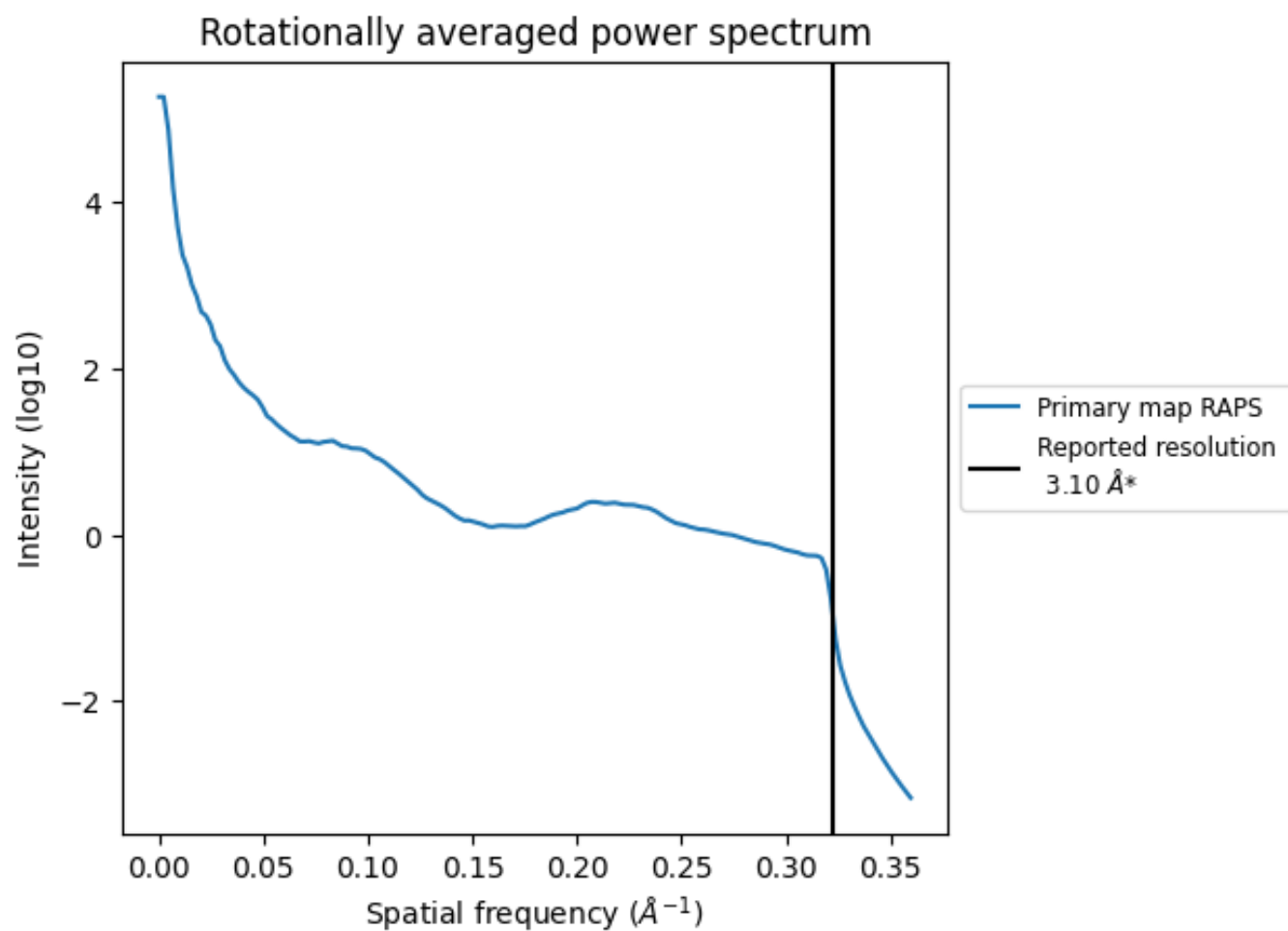
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 459 nm³; this corresponds to an approximate mass of 414 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

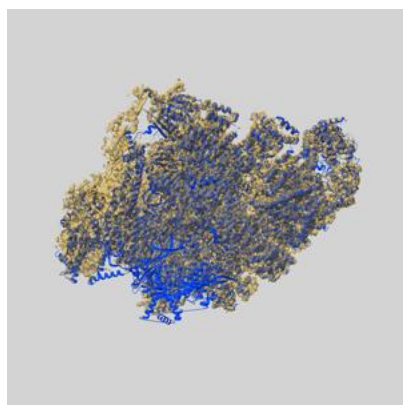
8 Fourier-Shell correlation ⓘ

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

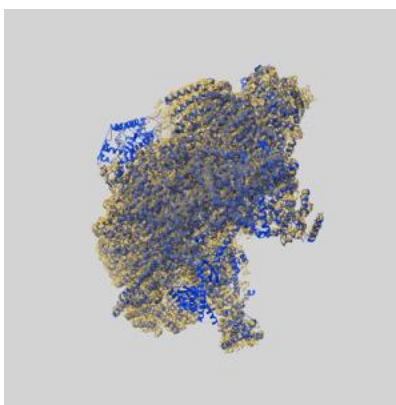
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10175 and PDB model 6SG9. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

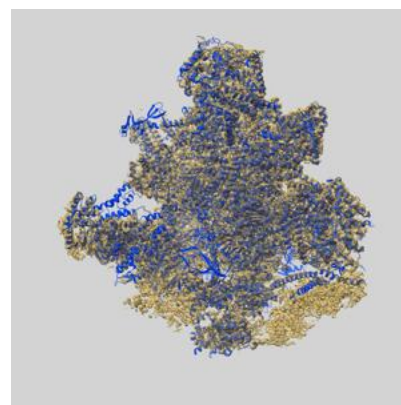
9.1 Map-model overlay [i](#)



X



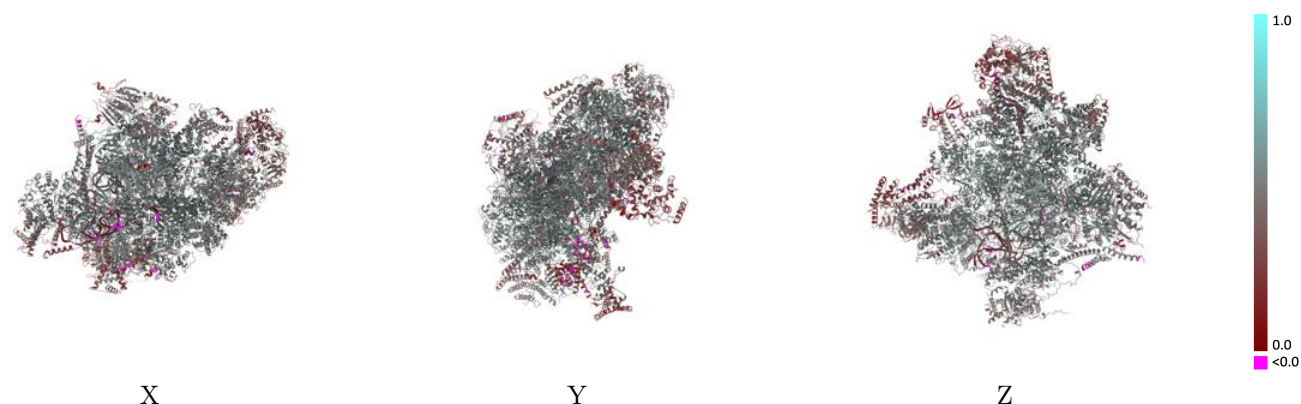
Y



Z

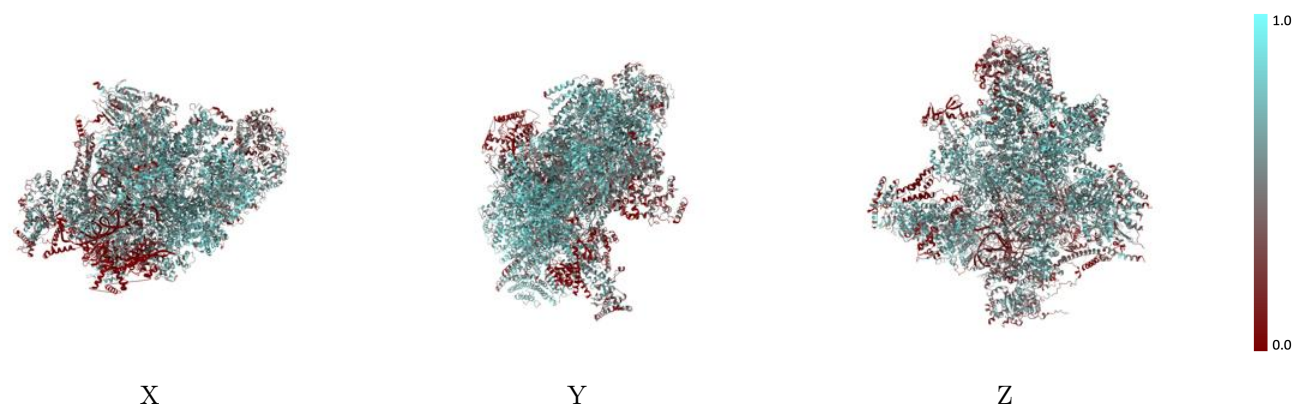
The images above show the 3D surface view of the map at the recommended contour level 0.0793 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



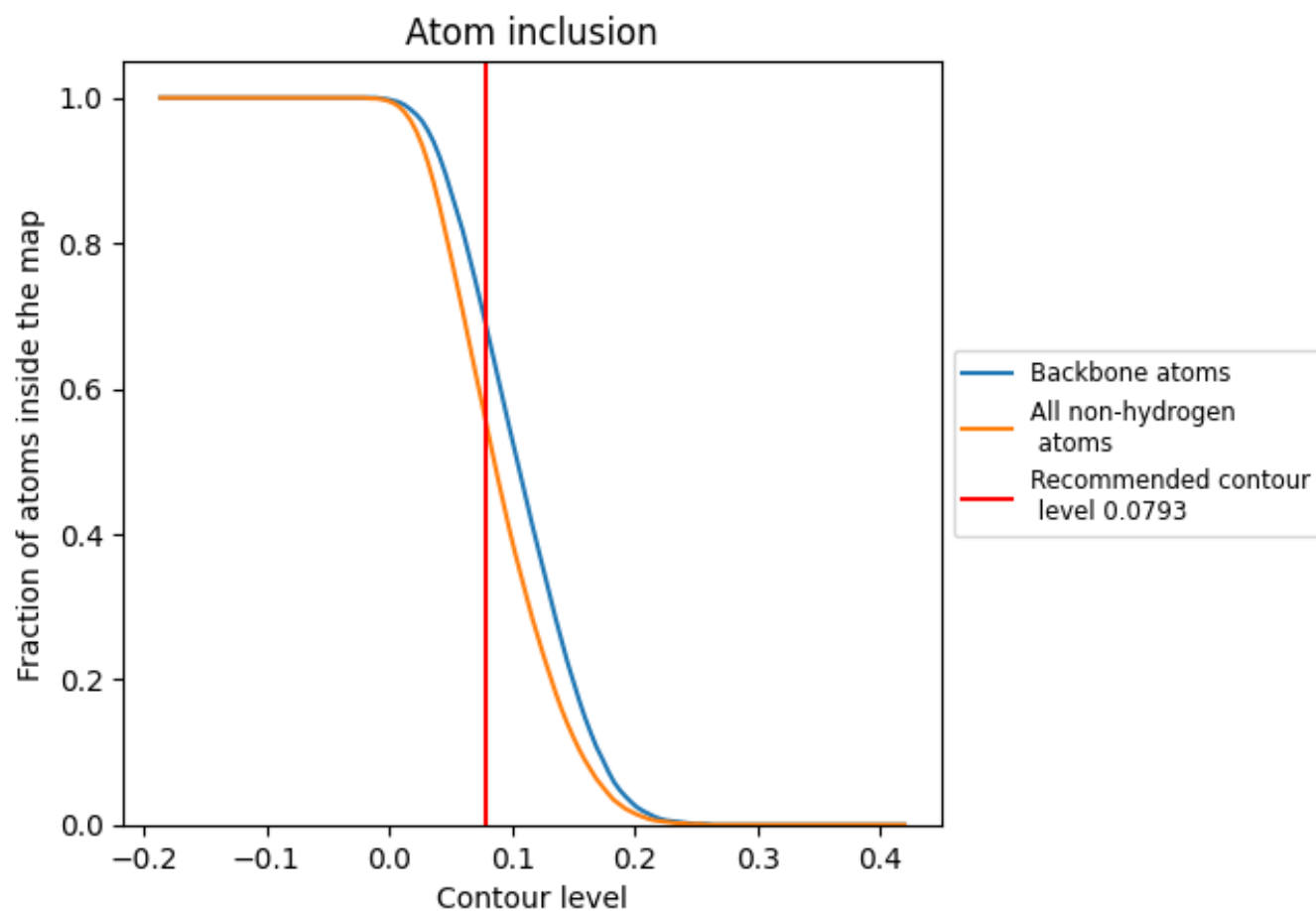
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0793).

9.4 Atom inclusion [i](#)



At the recommended contour level, 68% 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 (0.0793) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5480	0.4610
CA	0.3180	0.3180
CC	0.5390	0.5120
CE	0.4510	0.4920
CI	0.5420	0.4770
CJ	0.6350	0.5040
CK	0.5930	0.4770
CN	0.3020	0.4910
CS	0.0160	0.4150
Cg	0.7400	0.5020
CgA	0.9380	0.4720
CgB	1.0000	0.5320
Ci	0.5200	0.5180
Ck	0.5750	0.4440
Cn	0.3130	0.5000
DB	0.4570	0.4230
DC	0.6000	0.4420
DE	0.4310	0.3500
DF	0.6410	0.4960
DG	0.6500	0.4450
DH	0.6180	0.5060
DJ	0.6700	0.4990
DK	0.6350	0.4890
DT	0.7200	0.5410
DV	0.5620	0.4940
DW	0.5450	0.4600
DX	0.2540	0.4300
DY	0.5320	0.4670
F1	0.5000	0.4740
F1A	1.0000	0.6220
F1B	0.3080	0.5250
F4	0.4670	0.4220
FD	0.6730	0.4940
FF	0.4800	0.4620
FFA	0.3080	0.4450



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Chain	Atom inclusion	Q-score
FG	 0.7210	 0.5170
FGA	 1.0000	 0.7780
FH	 0.6410	 0.5000
FI	 0.6270	 0.5200
FJ	 0.4410	 0.4760
FK	 0.5910	 0.5040
FL	 0.6140	 0.5310
FLA	 1.0000	 0.7440
FLB	 1.0000	 0.6060
FV	 0.6500	 0.5030
FY	 0.4310	 0.3760
Fa	 0.4350	 0.4890
Fe	 0.6330	 0.5030
FeA	 1.0000	 0.4100
Ua	 0.4180	 0.4280
Ub	 0.2660	 0.4360
Uc	 0.2220	 0.4390
Ud	 0.5710	 0.4040
Ue	 0.1950	 0.3470
Uf	 0.4810	 0.5200
Ug	 0.4620	 0.2980
Uh	 0.0330	 0.3480
Ui	 0.5570	 0.3940
Uj	 0.4210	 0.4160
Uk	 0.5310	 0.4780
Ul	 0.2020	 0.2770
Um	 0.4550	 0.4370
Ux	 0.0050	 0.3290