



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 09:34 AM UTC

PDB ID : 6FEC / pdb_00006fec
EMDB ID : EMD-4242
Title : Human cap-dependent 48S pre-initiation complex
Authors : Schaffitzel, C.; Schaffitzel, C.
Deposited on : 2017-12-31
Resolution : 6.30 Å (reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

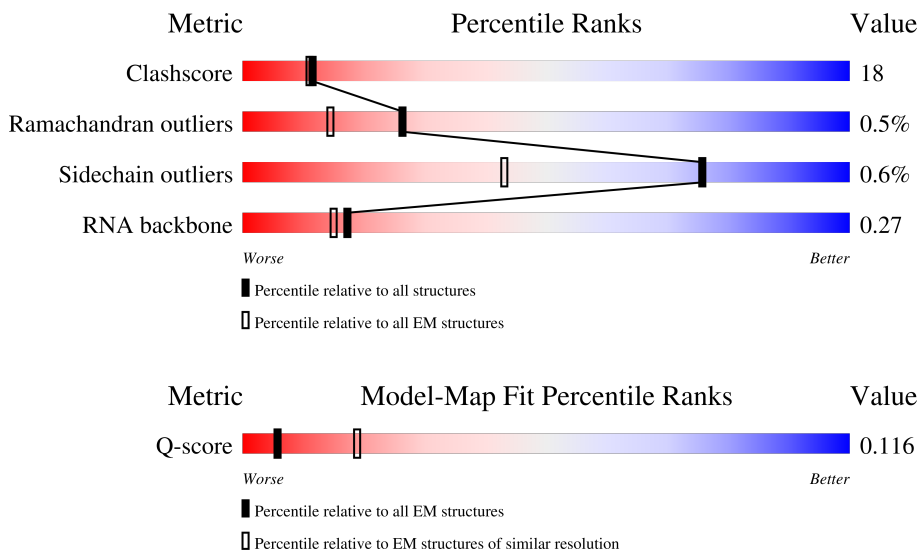
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 6.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	550 (5.80 - 6.80)

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

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1	1	1362	
2	2	843	
3	3	445	

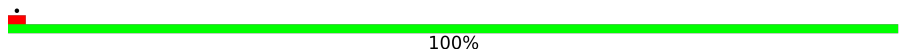
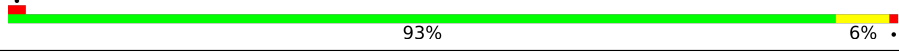
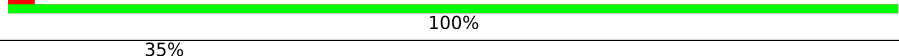
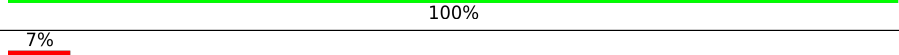
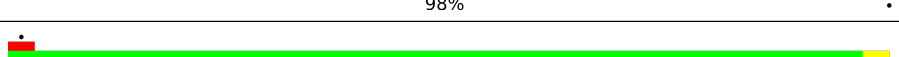
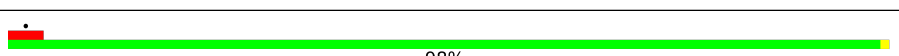
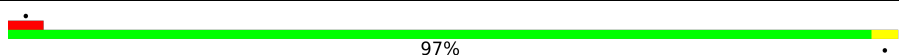
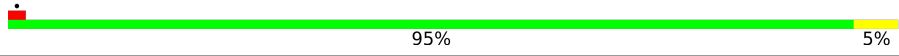
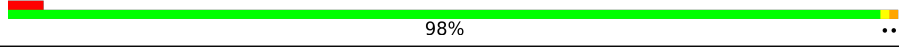
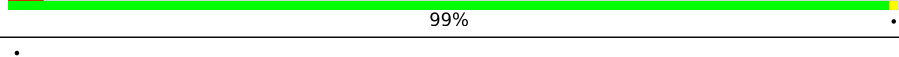
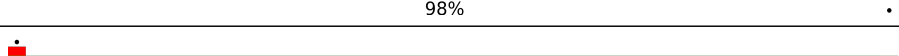
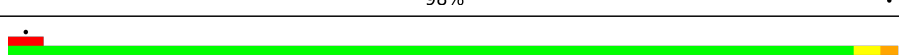
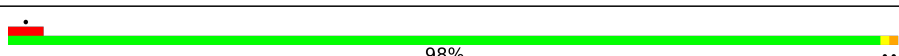
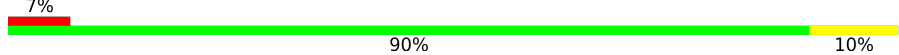
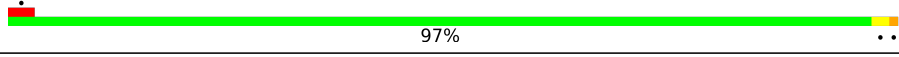
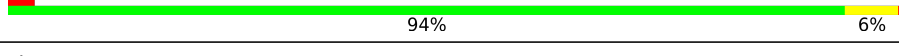
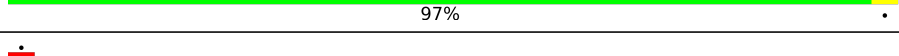
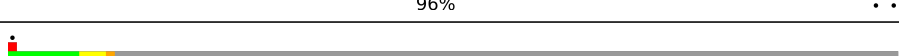




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Mol	Chain	Length	Quality of chain
4	4	364	39% 34% 25% 7%
5	5	352	57% 34% 8% 7%
6	6	218	57% 41%
7	7	564	43% 22% 34%
8	8	374	52% 44%
9	9	368	60% 36% 9%
10	A	1776	59% 41%
11	F	26	46% 54% 12%
12	G	158	96% 8%
13	H	141	98% 6%
14	I	263	98%
15	J	53	100% 13%
16	K	182	99%
17	L	137	96%
18	N	75	71% 29%
19	P	266	93% 6% 27%
20	Q	142	100% 6%
21	R	141	99%
22	S	422	99% 27%
23	U	191	96% 6%
24	V	59	90% 8%
25	W	75	96%
26	X	190	94% 5% 5%
27	Y	84	98% 5%
28	Z	150	99%

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Mol	Chain	Length	Quality of chain
29	a	129	 100%
30	b	82	 93% 6%
31	c	226	 100%
32	d	17	 35% 100%
33	e	126	 7% 98%
34	f	208	 96%
35	g	227	 98%
36	h	104	 97%
37	i	215	 95% 5%
38	j	136	 98%
39	k	99	 99%
40	l	64	 98%
41	m	313	 98%
42	n	127	 95%
43	o	206	 98%
44	p	71	 7% 90% 10%
45	q	237	 97%
46	r	124	 94% 6%
47	s	131	 97%
48	t	98	 96%
49	u	636	 8% 88%
50	w	1121	 25% 27% 9% 64%

2 Entry composition

There are 51 unique types of molecules in this entry. The entry contains 117189 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 Eukaryotic translation initiation factor 3 subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	600	4935	3107	893	914	21	0	1

- Molecule 2 is a protein called Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	2	558	4529	2842	805	849	33	0	1

- Molecule 3 is a protein called Eukaryotic translation initiation factor 3 subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	3	420	3466	2220	587	639	20	0	1

- Molecule 4 is a protein called Eukaryotic translation initiation factor 3 subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	4	272	2111	1330	359	410	12	0	0

- Molecule 5 is a protein called Eukaryotic translation initiation factor 3 subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	5	324	2624	1654	452	503	15	0	0

- Molecule 6 is a protein called Eukaryotic translation initiation factor 3 subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	6	216	1738	1109	286	330	13	0	1

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
6	166	THR	SER	conflict	UNP Q9UBQ5
6	172	MET	VAL	conflict	UNP Q9UBQ5

- Molecule 7 is a protein called Eukaryotic translation initiation factor 3 subunit L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	7	373	3110	2010	520	563	17	0	1

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
7	13	VAL	ALA	conflict	UNP Q9Y262
7	53	ARG	LYS	conflict	UNP Q9Y262
7	117	THR	ALA	conflict	UNP Q9Y262
7	151	ALA	GLU	conflict	UNP Q9Y262
7	430	SER	ASN	conflict	UNP Q9Y262

- Molecule 8 is a protein called Eukaryotic translation initiation factor 3 subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	8	366	2919	1850	494	558	17	0	1

- Molecule 9 is a protein called EUKARYOTIC TRANSLATION INITIATION FACTOR 3 SUBUNIT D.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	9	356	2867	1804	500	548	15	0	0

- Molecule 10 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
10	A	1776	37881	16910	6782	12414	1775	0	0

- Molecule 11 is a RNA chain called Messenger RNA (26-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	26	Total	C	N	O	P	0	0
			544	245	95	179	25		

- Molecule 12 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	158	Total	C	N	O	S	0	0
			1296	827	241	221	7		

- Molecule 13 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	141	Total	C	N	O	S	0	0
			1124	715	212	194	3		

- Molecule 14 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	263	Total	C	N	O	S	0	0
			2083	1329	385	359	10		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	25	SER	GLY	conflict	UNP P62701
I	51	LYS	ARG	conflict	UNP P62701
I	78	ALA	THR	conflict	UNP P62701
I	156	MET	VAL	conflict	UNP P62701

- Molecule 15 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	53	Total	C	N	O	S	0	0
			445	278	90	72	5		

- Molecule 16 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	182	Total	C	N	O	S	0	0
			1499	952	300	245	2		

- Molecule 17 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	137	Total	C	N	O	S	0	0
			1140	714	231	194	1		

- Molecule 18 is a RNA chain called Transfer RNA (75-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	75	Total	C	N	O	P	0	0
			1604	717	298	515	74		

- Molecule 19 is a protein called Eukaryotic translation initiation factor 2 subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	266	Total	C	N	O	S	0	0
			2147	1354	376	406	11		

- Molecule 20 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	142	Total	C	N	O	S	0	0
			1107	698	220	185	4		

- Molecule 21 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	R	141	Total	C	N	O	S	0	0
			1113	701	213	196	3		

- Molecule 22 is a protein called Eukaryotic translation initiation factor 2 subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S	422	Total	C	N	O	S	0	0
			3214	2044	561	592	17		

- Molecule 23 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	191	Total	C	N	O	S	0	0
			1509	943	286	273	7		

- Molecule 24 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	V	59	473	293	104	75	1	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	83	VAL	ALA	conflict	UNP P62861
V	91	LEU	PRO	conflict	UNP P62861
V	102	ARG	LYS	conflict	UNP P62861

- Molecule 25 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	W	75	599	382	111	105	1	0	0

- Molecule 26 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	X	190	1530	975	281	273	1	0	0

- Molecule 27 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	Y	84	659	413	122	116	8	0	0

- Molecule 28 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	Z	150	1208	773	229	205	1	0	0

- Molecule 29 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	a	129	1034	659	193	176	6	0	0

- Molecule 30 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	b	82	620	378	117	120	5	0	0

- Molecule 31 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	c	226	1743	1127	300	307	9	0	0

- Molecule 32 is a protein called EUKARYOTIC TRANSLATION INITIATION FACTOR 2 BETA SUBUNIT (eIF2-Beta).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	d	17	147	94	22	30	1	0	0

- Molecule 33 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	e	126	1020	639	188	188	5	0	0

- Molecule 34 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	f	208	1643	1045	289	301	8	0	0

- Molecule 35 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	g	227	1765	1124	317	316	8	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	195	SER	THR	conflict	UNP P23396

- Molecule 36 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	h	104	822	514	156	148	4	0	0

- Molecule 37 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	i	215	1742	1107	309	311	15	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
i	136	HIS	ARG	conflict	UNP P61247
i	146	CYS	ARG	conflict	UNP P61247

- Molecule 38 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	j	136	1016	621	199	190	6	0	0

- Molecule 39 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	k	99	790	491	162	131	6	0	0

- Molecule 40 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	l	64	507	308	102	95	2	0	0

- Molecule 41 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	m	313	2437	1535	424	466	12	0	0

- Molecule 42 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	n	127	1061	673	201	180	7	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	46	SER	ASN	conflict	UNP P62841

- Molecule 43 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	o	206	1680	1054	329	292	5	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
o	47	GLY	ARG	conflict	UNP P62241

- Molecule 44 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	p	71	582	367	109	99	7	0	0

- Molecule 45 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	q	237	1924	1200	387	330	7	0	0

- Molecule 46 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	r	124	958	600	170	179	9	0	0

- Molecule 47 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	s	131	1065	673	206	181	5	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
s	41	GLN	ARG	conflict	UNP P62847

- Molecule 48 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	t	98	828	539	148	135	6	0	0

- Molecule 49 is a protein called Eukaryotic translation initiation factor 4B.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
49	u	76	608	385	104	119	0	0

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
u	-119	MET	-	initiating methionine	UNP P23588
u	-118	SER	-	expression tag	UNP P23588
u	-117	TYR	-	expression tag	UNP P23588
u	-116	TYR	-	expression tag	UNP P23588
u	-115	HIS	-	expression tag	UNP P23588
u	-114	HIS	-	expression tag	UNP P23588
u	-113	HIS	-	expression tag	UNP P23588
u	-112	HIS	-	expression tag	UNP P23588
u	-111	HIS	-	expression tag	UNP P23588
u	-110	HIS	-	expression tag	UNP P23588
u	-109	ASP	-	expression tag	UNP P23588
u	-108	TYR	-	expression tag	UNP P23588
u	-107	ASP	-	expression tag	UNP P23588
u	-106	ILE	-	expression tag	UNP P23588
u	-105	PRO	-	expression tag	UNP P23588
u	-104	THR	-	expression tag	UNP P23588
u	-103	THR	-	expression tag	UNP P23588
u	-102	GLU	-	expression tag	UNP P23588
u	-101	ASN	-	expression tag	UNP P23588
u	-100	LEU	-	expression tag	UNP P23588
u	-99	TYR	-	expression tag	UNP P23588
u	-98	PRO	-	expression tag	UNP P23588
u	-97	GLN	-	expression tag	UNP P23588
u	-96	GLY	-	expression tag	UNP P23588

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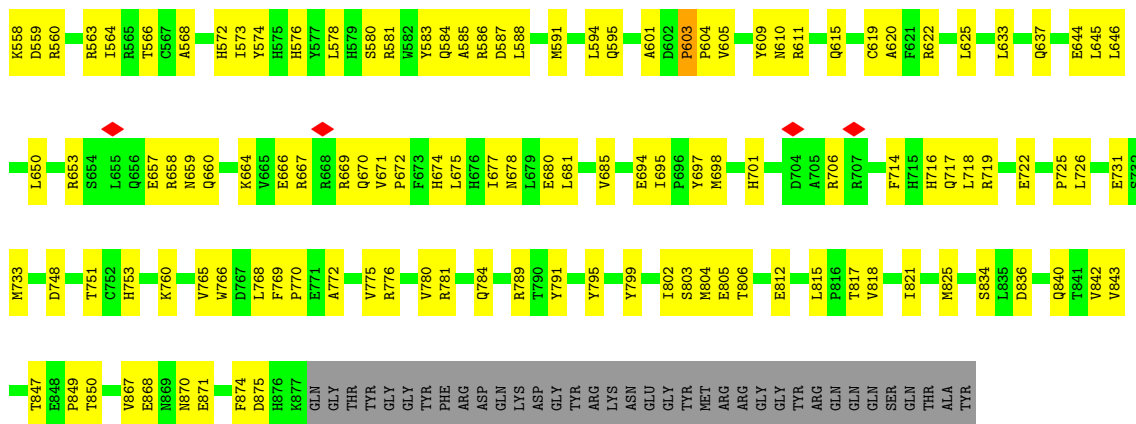
Chain	Residue	Modelled	Actual	Comment	Reference
u	-95	ALA	-	expression tag	UNP P23588

- Molecule 50 is a protein called Eukaryotic translation initiation factor 3 subunit B.

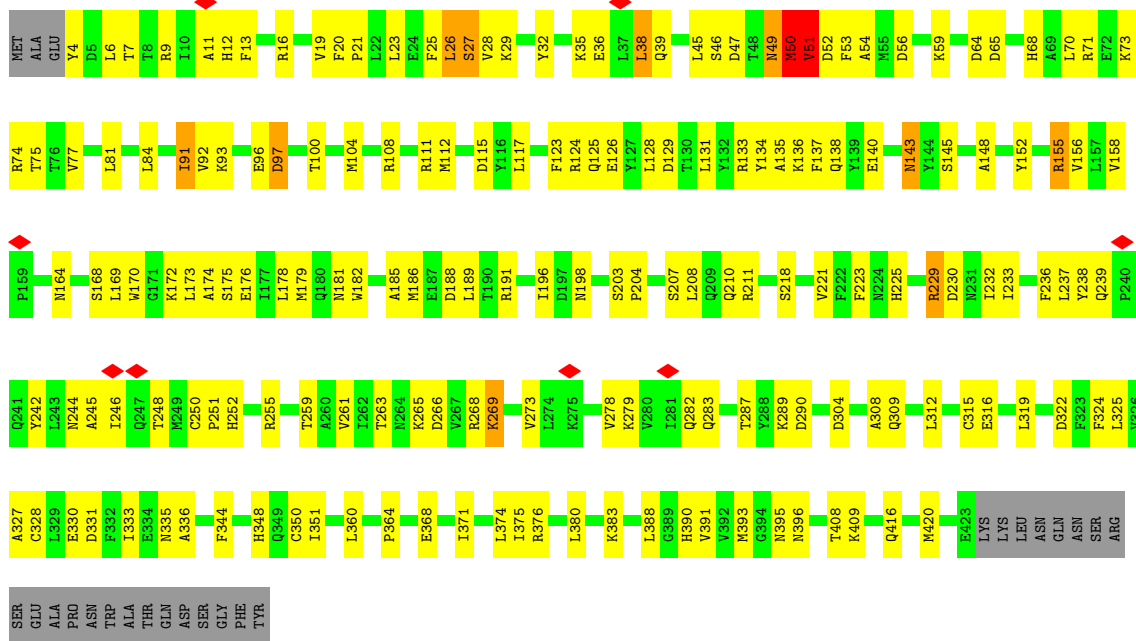
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	w	403	3308	2132	573	587	16	0	0

- Molecule 51 is water.

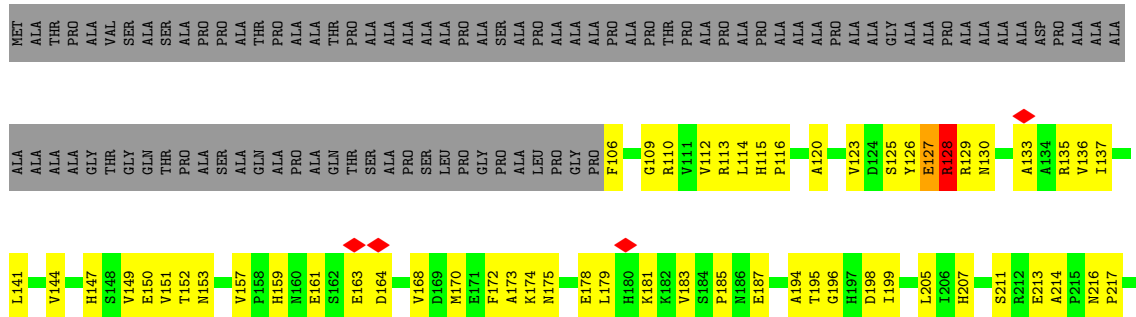
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
51	1	1	1	1	0
51	9	376	376	376	0
51	A	6	6	6	0
51	H	5	5	5	0
51	U	13	13	13	0
51	j	1	1	1	0
51	l	8	8	8	0
51	m	5	5	5	0

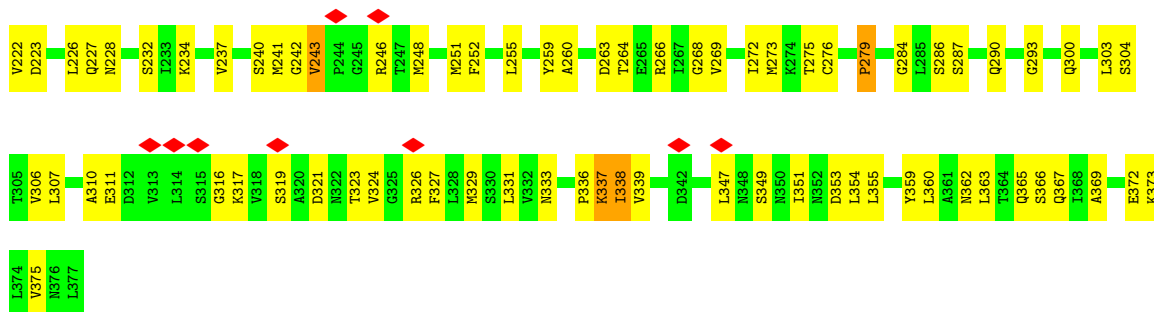


• Molecule 3: Eukaryotic translation initiation factor 3 subunit E

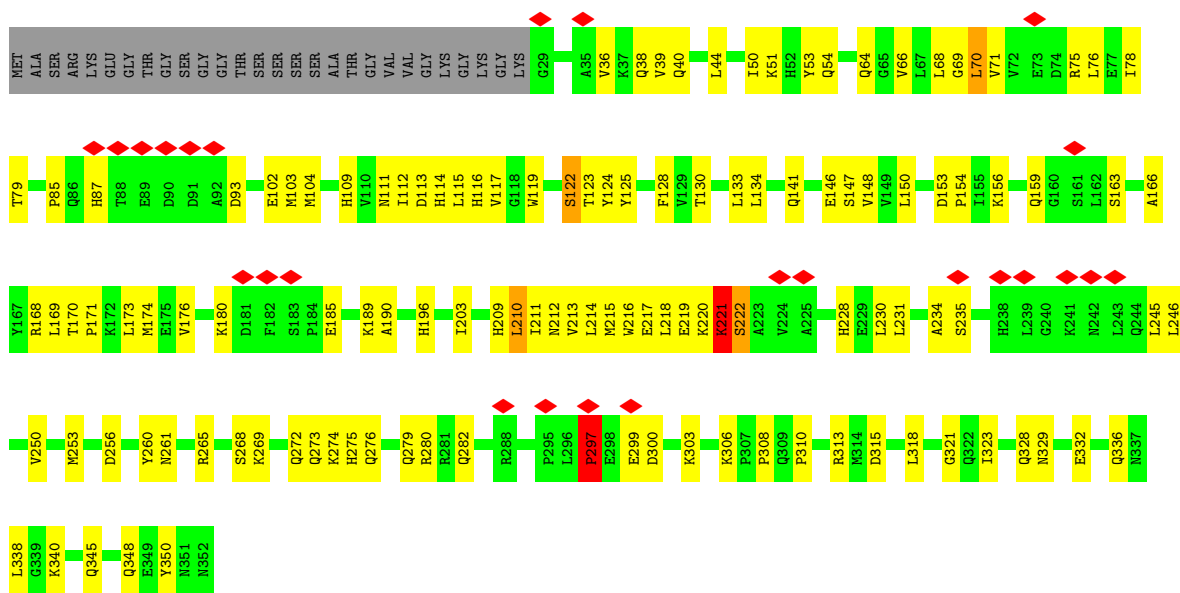


• Molecule 4: Eukaryotic translation initiation factor 3 subunit F

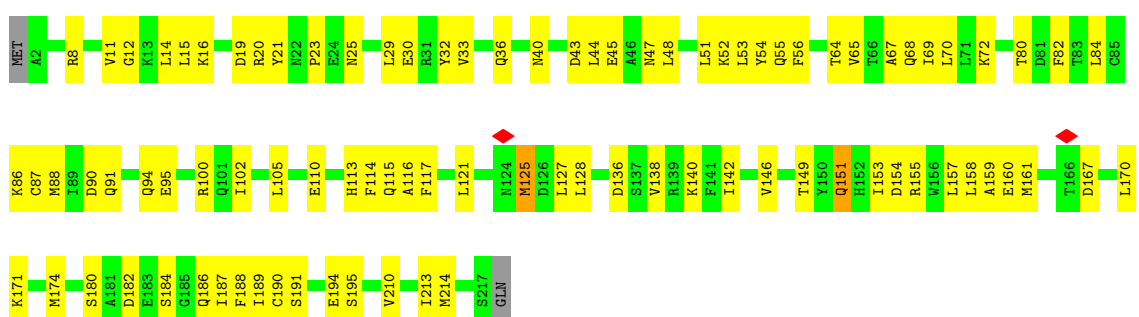




• Molecule 5: Eukaryotic translation initiation factor 3 subunit H

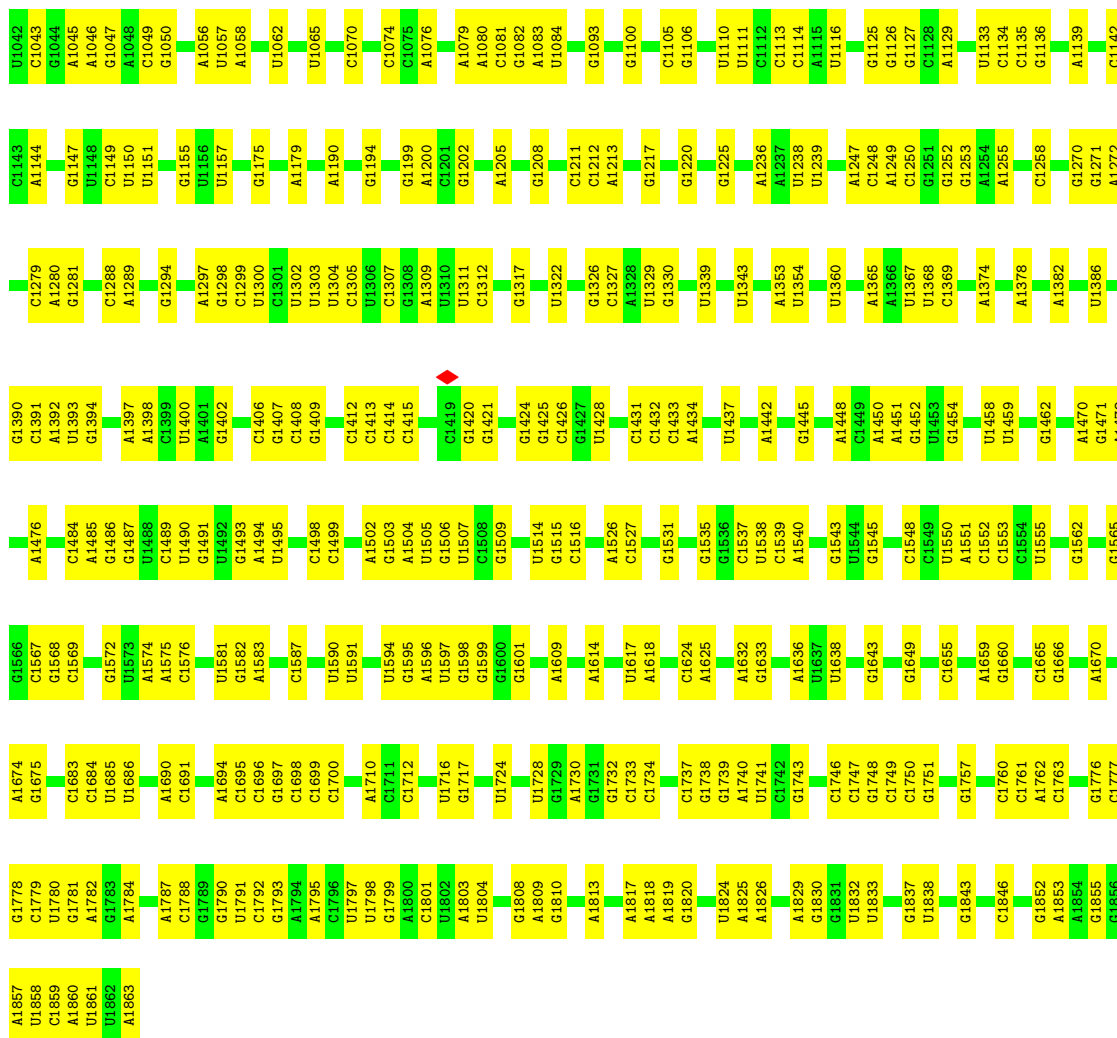


• Molecule 6: Eukaryotic translation initiation factor 3 subunit K

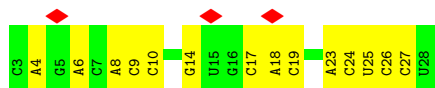


• Molecule 7: Eukaryotic translation initiation factor 3 subunit L

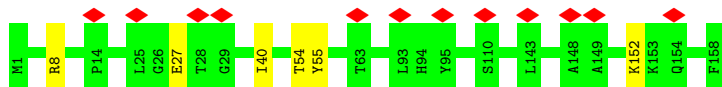




• Molecule 11: Messenger RNA (26-MER)

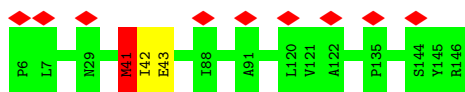


• Molecule 12: 40S ribosomal protein S11



• Molecule 13: 40S ribosomal protein S16

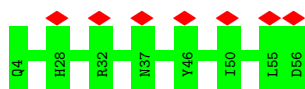




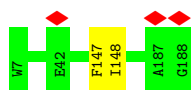
- Molecule 14: 40S ribosomal protein S4, X isoform



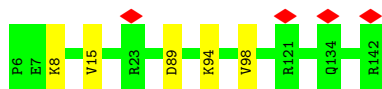
- Molecule 15: 40S ribosomal protein S29



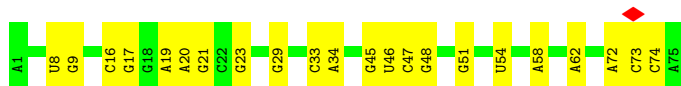
- Molecule 16: 40S ribosomal protein S9



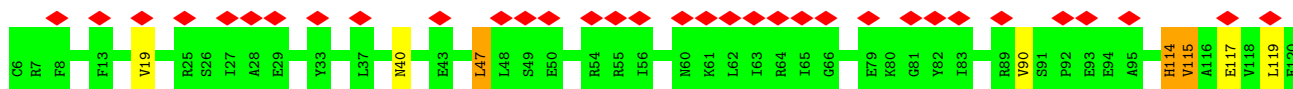
- Molecule 17: 40S ribosomal protein S18

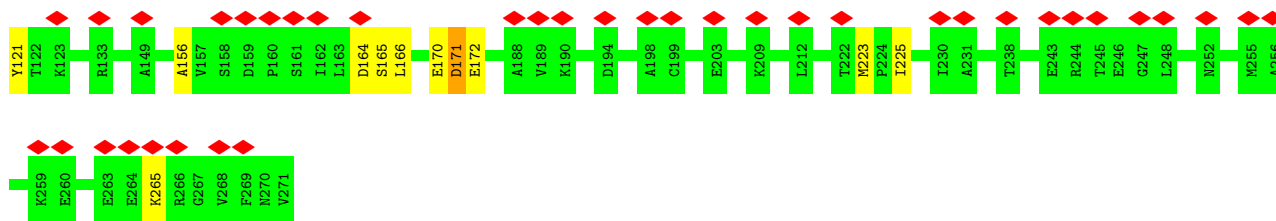


- Molecule 18: Transfer RNA (75-MER)

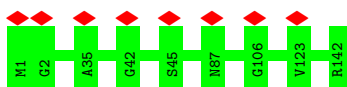


- Molecule 19: Eukaryotic translation initiation factor 2 subunit 1





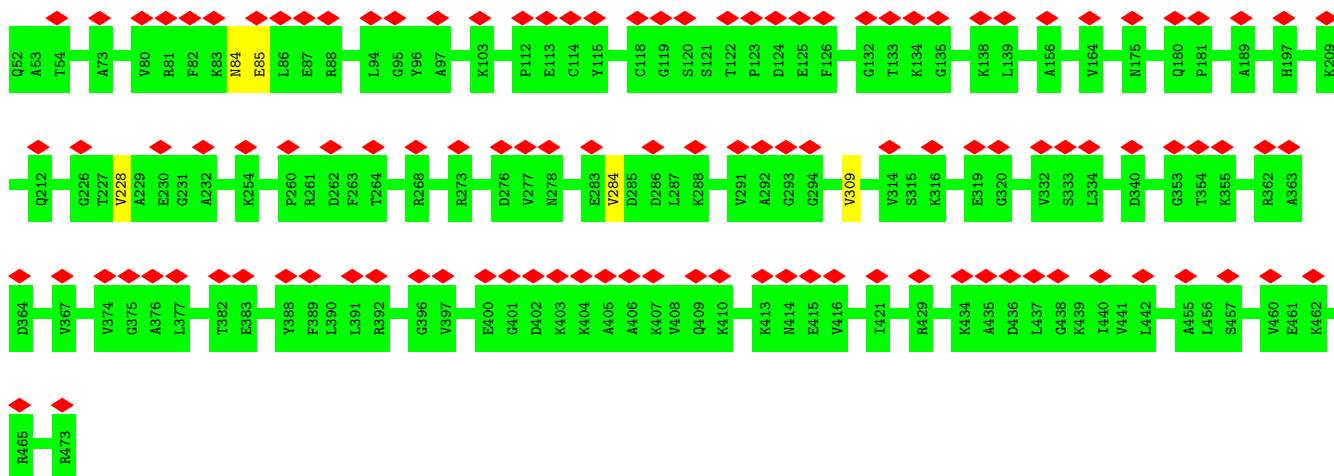
- Molecule 20: 40S ribosomal protein S23



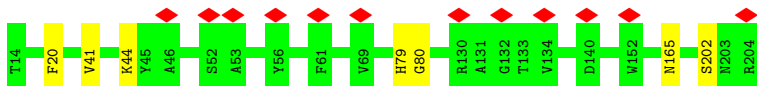
- Molecule 21: 40S ribosomal protein S19




- Molecule 22: Eukaryotic translation initiation factor 2 subunit 3

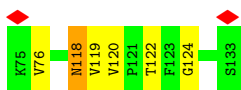


- Molecule 23: 40S ribosomal protein S5



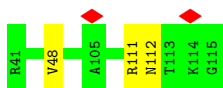
- Molecule 24: 40S ribosomal protein S30

Chain V:  90% 8%



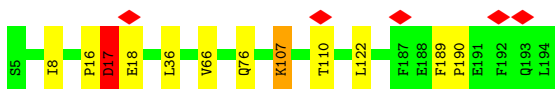
- Molecule 25: 40S ribosomal protein S25

Chain W:  96%



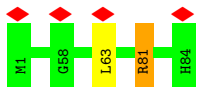
- Molecule 26: 40S ribosomal protein S7

Chain X:  94% 5%



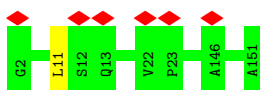
- Molecule 27: 40S ribosomal protein S27

Chain Y:  5% 98%



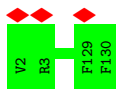
- Molecule 28: 40S ribosomal protein S13

Chain Z:  99%

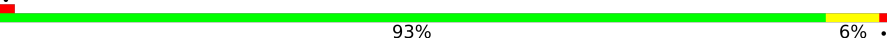


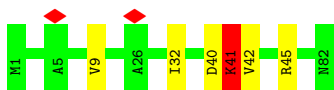
- Molecule 29: 40S ribosomal protein S15a

Chain a:  100%

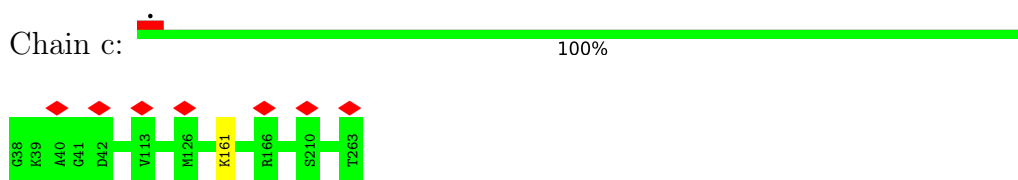


- Molecule 30: 40S ribosomal protein S21

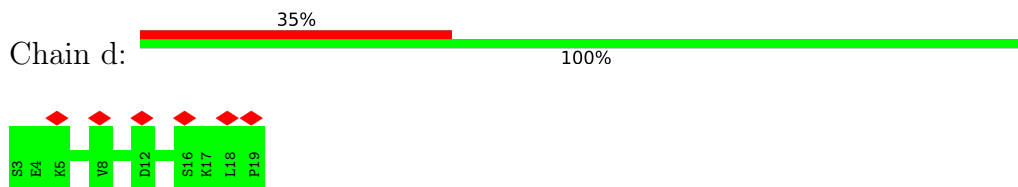
Chain b:  93% 6%



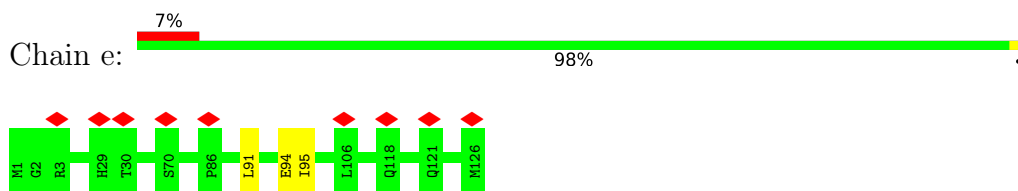
- Molecule 31: 40S ribosomal protein S2



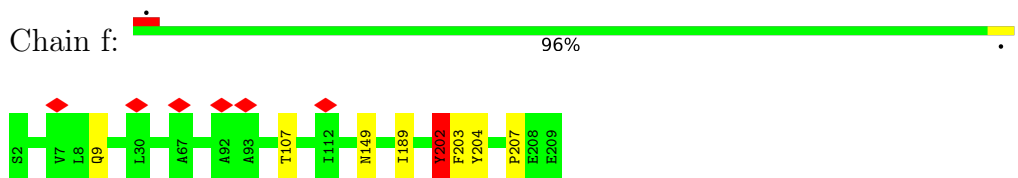
- Molecule 32: EUKARYOTIC TRANSLATION INITIATION FACTOR 2 BETA SUBUNIT (eIF2-Beta)



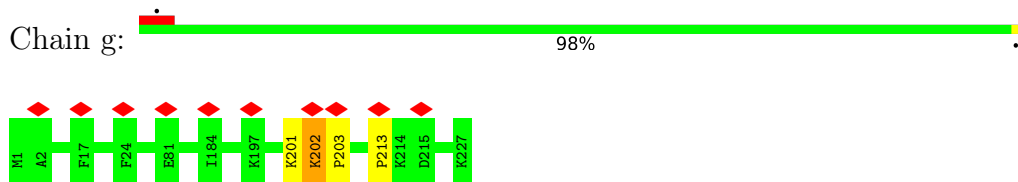
- Molecule 33: 40S ribosomal protein S17



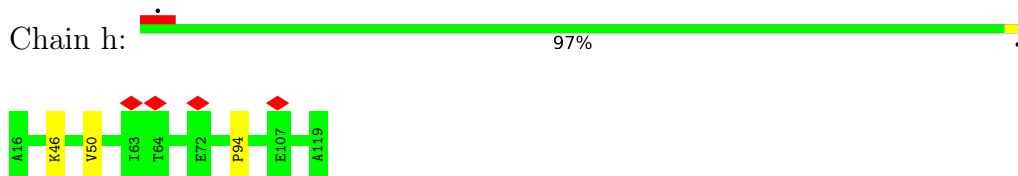
- Molecule 34: 40S ribosomal protein SA



- Molecule 35: 40S ribosomal protein S3

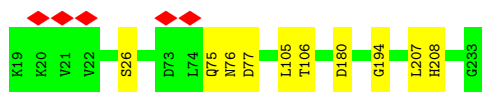


- Molecule 36: 40S ribosomal protein S20

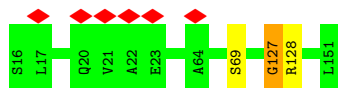


- Molecule 37: 40S ribosomal protein S3a

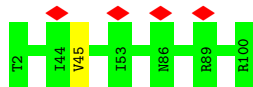




- Molecule 38: 40S ribosomal protein S14



- Molecule 39: 40S ribosomal protein S26



- Molecule 40: 40S ribosomal protein S28



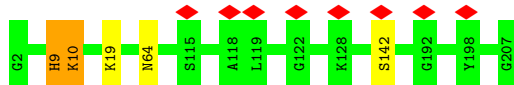
- Molecule 41: Receptor of activated protein C kinase 1



- Molecule 42: 40S ribosomal protein S15



- Molecule 43: 40S ribosomal protein S8



- Molecule 44: Ubiquitin-40S ribosomal protein S27a

W263	W264	G265	E266	K267	F268	K269	Q270	I271	Q272	R273	F274	S275	H276	Q277	G278	V279	Q280	L281	I282	D283	F284	S285	P286	C287	E288	R289	Y290	L291	Y292	I293	F294	S295	P296	L297	M298	D299	T300	Q301	D302	D303	A306	I307	I308	I309	W310	D311	I312	L313	T314	G315	H316	K317	K318	R319	E324	S325	S326	A327	H328	W329	P330	I331	F332	K333	W334	S335	H336	D337	G338	K339	F340	F341	A342	R343	M344	T345	L346	D347	T348	L349	S350	I351	Y352	E353	T354	P355	S356	M357	L360	D361	K362	K363	S364	L365	K366	I367	S368	G369	I370	K371	D372	F373	S374	W375	S376	P377	G378	G379	N380	I381	I382	A383	F384	W385	E388	D389	K390	D391	I392	P393	A394	R395	S396	T397	L398	M399	Q400	L401	P402	S403	R404	Q405	E406	I407	R408	V409	R410	M411	L412	F413	M414	V415	V416	D417	C418	K419	L420	H421	K422	V433	T436	P437	Q441	G442	M446	F447	E448	I449	F450	R451	M452	R453	E454	K455	Q456	D460	V461	V462	E463	M464	K465	E466	T467	I468	I469	A470	F471	A472	W473	E474	P475	N476	G477	A481	V482	L483	H484	G485	E486	A487	P488	R489	I490	S491	V492	S493	F494	Y495	H496	V497	K498	S499	M500	G501	K502	I503	E504	L505	S506	K507	M508	F509	D510	K511	Q512	Q513	A514	N515	W519	S520	P521	Q522	G523	Q524	F525	V526	A529	G530	R532	S533	M534	N535	G536	A537	L538	A539	F540	V541	D542	T543	S544	D545	C546	T547	V548	M549	N550	I551	A552	E553	H554	Y555	M556	A557	S558	D559	V560	E561	W562	D563	P564	T565	G566	R567	Y568	V569	S572	V573	S574	S577	H578	K579	V580	D581	N582	A583	Y584	L586	L587	T588	F589	Q590	G591	R592	L593	L594	Q595	K596	N597	N598	K599	D600	R601	F602	C603	M607	R608	P609	R610	PRO	PRO	THR	LEU	LEU	LEU	SER	GLN	GLY	VAL	ASP	THR	LYS	ASP	GLN	ILE	LEU	ASP	SER	ASN	VAL	LYS	ASP	TYR	SER	GLU	ILE	PHE	GLU	ILE	GLN	LYS	ARG	LEU	SER	GLN	SER	LYS	ALA	SER	THR	GLU	VAL
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	50604	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	112000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.544	Depositor
Minimum map value	-0.322	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	520.0, 520.0, 520.0	wwPDB
Map dimensions	208, 208, 208	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.5, 2.5, 2.5	Depositor

5 Model quality

5.1 Standard geometry

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	1	0.32	0/5021	0.75	5/6781 (0.1%)
2	2	0.29	0/4608	0.75	10/6219 (0.2%)
3	3	0.34	2/3539 (0.1%)	0.90	17/4788 (0.4%)
4	4	0.31	0/2149	0.81	7/2920 (0.2%)
5	5	0.31	0/2675	0.85	10/3609 (0.3%)
6	6	0.28	0/1773	0.74	4/2398 (0.2%)
7	7	0.30	0/3186	0.80	9/4298 (0.2%)
8	8	0.31	0/2964	0.90	14/4000 (0.3%)
9	9	0.24	0/2921	0.61	0/3957
10	A	0.29	0/42353	0.52	3/66010 (0.0%)
11	F	0.17	0/606	0.36	0/941
12	G	0.34	0/1319	0.84	6/1761 (0.3%)
13	H	0.29	0/1142	0.80	2/1528 (0.1%)
14	I	0.30	0/2125	0.78	5/2856 (0.2%)
15	J	0.28	0/455	0.74	0/603
16	K	0.28	0/1523	0.71	0/2031
17	L	0.32	0/1158	0.80	0/1548
18	N	0.23	0/1795	0.43	0/2798
19	P	0.34	1/2178 (0.0%)	0.96	10/2935 (0.3%)
20	Q	0.27	0/1125	0.72	0/1500
21	R	0.31	0/1133	0.72	0/1517
22	S	0.29	0/3267	0.73	3/4415 (0.1%)
23	U	0.27	0/1531	0.74	4/2059 (0.2%)
24	V	0.30	0/478	1.06	7/628 (1.1%)
25	W	0.33	0/605	0.81	0/810
26	X	0.34	0/1553	0.92	5/2079 (0.2%)
27	Y	0.32	0/673	0.80	3/902 (0.3%)
28	Z	0.27	0/1232	0.63	0/1656
29	a	0.24	0/1051	0.60	0/1406
30	b	0.30	0/627	0.91	4/839 (0.5%)
31	c	0.29	0/1779	0.65	0/2399
32	d	0.17	0/149	0.44	0/197
33	e	0.29	0/1032	0.76	2/1383 (0.1%)
34	f	0.32	0/1680	0.88	5/2283 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	g	0.31	0/1793	0.70	2/2412 (0.1%)
36	h	0.29	0/832	0.80	2/1117 (0.2%)
37	i	0.32	0/1770	0.83	5/2367 (0.2%)
38	j	0.30	0/1029	0.79	4/1380 (0.3%)
39	k	0.26	0/803	0.74	2/1076 (0.2%)
40	l	0.33	0/509	0.72	0/680
41	m	0.35	0/2494	0.74	3/3394 (0.1%)
42	n	0.33	0/1080	0.90	3/1437 (0.2%)
43	o	0.38	0/1709	0.87	4/2278 (0.2%)
44	p	0.41	0/594	1.02	2/786 (0.3%)
45	q	0.30	0/1947	0.76	2/2590 (0.1%)
46	r	0.35	0/968	0.84	2/1296 (0.2%)
47	s	0.37	0/1083	0.83	3/1437 (0.2%)
48	t	0.33	0/852	0.93	2/1147 (0.2%)
49	u	0.33	0/619	0.98	4/836 (0.5%)
50	w	0.24	0/3407	0.80	6/4620 (0.1%)
All	All	0.30	3/122894 (0.0%)	0.70	181/174907 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1	0	6
2	2	0	8
3	3	0	12
4	4	0	8
5	5	0	4
7	7	0	4
8	8	0	8
9	9	0	3
12	G	0	1
13	H	0	2
14	I	0	2
16	K	0	1
17	L	0	3
19	P	0	11
22	S	0	1
23	U	0	2
24	V	0	1
25	W	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
26	X	0	5
27	Y	0	1
30	b	0	2
31	c	0	1
33	e	0	1
34	f	0	4
35	g	0	2
36	h	0	2
37	i	0	6
38	j	0	1
41	m	0	3
42	n	0	4
43	o	0	2
44	p	0	6
45	q	0	4
46	r	0	4
48	t	0	3
49	u	0	1
50	w	0	1
All	All	0	132

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	P	115	VAL	CA-C	5.95	1.58	1.53
3	3	20	PHE	C-N	5.54	1.38	1.33
3	3	75	THR	CA-C	-5.01	1.46	1.52

All (181) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	w	562	TRP	CA-C-N	14.30	146.38	122.65
50	w	562	TRP	C-N-CA	14.30	146.38	122.65
14	I	13	ALA	CA-C-N	12.53	147.04	121.48
14	I	13	ALA	C-N-CA	12.53	147.04	121.48
50	w	211	VAL	N-CA-C	11.30	124.18	108.93
19	P	114	HIS	CA-C-N	11.16	133.56	122.96
19	P	114	HIS	C-N-CA	11.16	133.56	122.96
3	3	268	ARG	CA-C-N	10.36	140.36	121.70
3	3	268	ARG	C-N-CA	10.36	140.36	121.70
8	8	115	LYS	CA-C-N	9.92	139.55	121.70
8	8	115	LYS	C-N-CA	9.92	139.55	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	7	348	SER	CA-C-N	9.88	139.48	121.70
7	7	348	SER	C-N-CA	9.88	139.48	121.70
5	5	222	SER	N-CA-C	9.70	131.47	110.80
43	o	142	SER	CA-C-N	8.98	137.87	121.70
43	o	142	SER	C-N-CA	8.98	137.87	121.70
3	3	143	ASN	CA-C-N	8.50	136.99	121.70
3	3	143	ASN	C-N-CA	8.50	136.99	121.70
34	f	107	THR	N-CA-C	-8.40	104.17	114.75
26	X	8	ILE	N-CA-C	-8.26	105.27	113.20
50	w	210	SER	CA-C-N	8.23	132.79	120.77
50	w	210	SER	C-N-CA	8.23	132.79	120.77
26	X	17	ASP	N-CA-C	8.00	127.83	110.80
48	t	1	MET	CA-C-N	7.87	135.87	121.70
48	t	1	MET	C-N-CA	7.87	135.87	121.70
2	2	391	THR	CA-C-N	7.74	135.63	121.70
2	2	391	THR	C-N-CA	7.74	135.63	121.70
22	S	84	ASN	CA-C-N	7.67	135.51	121.70
22	S	84	ASN	C-N-CA	7.67	135.51	121.70
3	3	50	MET	CA-C-N	7.39	135.27	121.97
3	3	50	MET	C-N-CA	7.39	135.27	121.97
5	5	54	GLN	N-CA-C	-7.17	102.64	112.03
7	7	486	PHE	CA-C-N	7.06	134.41	121.70
7	7	486	PHE	C-N-CA	7.06	134.41	121.70
7	7	379	PRO	CA-C-N	7.02	134.34	121.70
7	7	379	PRO	C-N-CA	7.02	134.34	121.70
24	V	119	VAL	N-CA-C	6.95	123.81	109.34
4	4	279	PRO	CA-C-N	6.89	134.11	121.70
4	4	279	PRO	C-N-CA	6.89	134.11	121.70
47	s	86	GLU	N-CA-C	6.86	124.96	109.81
7	7	382	ILE	N-CA-C	-6.84	105.67	112.17
8	8	13	ASP	CA-C-N	6.80	133.94	121.70
8	8	13	ASP	C-N-CA	6.80	133.94	121.70
8	8	334	VAL	CA-C-N	6.80	134.52	121.54
8	8	334	VAL	C-N-CA	6.80	134.52	121.54
2	2	366	LEU	N-CA-C	-6.72	104.90	113.23
5	5	297	PRO	CA-C-N	6.58	133.54	121.70
5	5	297	PRO	C-N-CA	6.58	133.54	121.70
3	3	198	ASN	CA-C-N	6.55	133.48	121.70
3	3	198	ASN	C-N-CA	6.55	133.48	121.70
19	P	121	TYR	CA-C-N	6.54	133.48	121.70
19	P	121	TYR	C-N-CA	6.54	133.48	121.70
3	3	325	LEU	CA-C-N	-6.53	116.57	122.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	325	LEU	C-N-CA	-6.53	116.57	122.97
8	8	195	ASP	CA-C-N	6.49	133.39	121.70
8	8	195	ASP	C-N-CA	6.49	133.39	121.70
37	i	26	SER	N-CA-C	-6.47	104.05	114.09
19	P	115	VAL	CA-C-N	6.45	133.32	121.70
19	P	115	VAL	C-N-CA	6.45	133.32	121.70
12	G	27	GLU	CA-C-N	6.45	133.31	121.70
12	G	27	GLU	C-N-CA	6.45	133.31	121.70
47	s	102	THR	CA-C-N	6.43	133.28	121.70
47	s	102	THR	C-N-CA	6.43	133.28	121.70
4	4	240	SER	CA-C-N	6.41	133.24	121.70
4	4	240	SER	C-N-CA	6.41	133.24	121.70
23	U	41	VAL	N-CA-C	-6.38	107.64	113.71
12	G	40	ILE	N-CA-C	-6.38	107.08	113.20
39	k	45	VAL	CA-C-N	6.36	130.16	120.82
39	k	45	VAL	C-N-CA	6.36	130.16	120.82
19	P	171	ASP	N-CA-C	-6.29	101.47	111.02
37	i	207	LEU	N-CA-C	6.23	118.20	110.91
24	V	118	ASN	CA-C-N	6.23	133.19	121.97
24	V	118	ASN	C-N-CA	6.23	133.19	121.97
49	u	17	ILE	N-CA-CB	-6.22	105.37	112.21
12	G	54	THR	CA-C-N	6.21	129.95	120.82
12	G	54	THR	C-N-CA	6.21	129.95	120.82
37	i	106	THR	CA-C-N	6.21	130.13	120.82
37	i	106	THR	C-N-CA	6.21	130.13	120.82
26	X	36	LEU	N-CA-C	-6.20	105.22	114.64
24	V	122	THR	N-CA-C	-6.19	106.70	114.56
42	n	12	PHE	N-CA-C	-6.18	106.06	113.97
13	H	41	MET	CA-C-N	6.17	133.07	121.97
13	H	41	MET	C-N-CA	6.17	133.07	121.97
19	P	115	VAL	CB-CA-C	6.13	117.42	111.23
26	X	110	THR	CA-C-N	6.12	130.93	121.19
26	X	110	THR	C-N-CA	6.12	130.93	121.19
24	V	76	VAL	N-CA-C	-6.12	107.53	113.53
12	G	55	TYR	N-CA-C	6.06	118.12	110.24
1	1	22	GLY	N-CA-C	-6.03	98.90	113.18
34	f	189	ILE	CA-C-N	5.95	132.90	121.54
34	f	189	ILE	C-N-CA	5.95	132.90	121.54
3	3	75	THR	CA-C-O	-5.92	114.76	120.92
33	e	91	LEU	CA-C-N	5.91	132.34	121.70
33	e	91	LEU	C-N-CA	5.91	132.34	121.70
19	P	119	LEU	CA-C-N	5.86	132.24	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	P	119	LEU	C-N-CA	5.86	132.24	121.70
2	2	490	LEU	CA-C-N	5.84	132.21	121.70
2	2	490	LEU	C-N-CA	5.84	132.21	121.70
10	A	141	A	C2'-C3'-O3'	5.83	118.24	109.50
37	i	194	GLY	N-CA-C	5.83	119.26	112.50
3	3	155	ARG	CA-C-N	5.82	128.74	120.53
3	3	155	ARG	C-N-CA	5.82	128.74	120.53
24	V	124	GLY	N-CA-C	5.81	118.80	112.29
50	w	215	SER	N-CA-C	5.74	118.27	110.06
46	r	118	SER	CA-C-N	5.68	132.40	121.54
46	r	118	SER	C-N-CA	5.68	132.40	121.54
27	Y	63	LEU	N-CA-C	-5.67	105.64	113.18
45	q	151	ASP	CA-C-N	5.66	132.34	121.54
45	q	151	ASP	C-N-CA	5.66	132.34	121.54
1	1	218	ILE	N-CA-C	-5.61	107.02	112.29
38	j	127	GLY	CA-C-N	5.59	132.21	121.54
38	j	127	GLY	C-N-CA	5.59	132.21	121.54
23	U	20	PHE	CA-C-N	5.56	126.26	120.03
23	U	20	PHE	C-N-CA	5.56	126.26	120.03
27	Y	81	ARG	CA-C-N	5.56	131.72	121.70
27	Y	81	ARG	C-N-CA	5.56	131.72	121.70
8	8	288	GLU	CA-C-N	5.54	131.67	121.70
8	8	288	GLU	C-N-CA	5.54	131.67	121.70
8	8	217	ALA	CA-C-N	5.50	132.04	121.54
8	8	217	ALA	C-N-CA	5.50	132.04	121.54
8	8	266	LEU	CA-C-N	5.49	131.58	121.70
8	8	266	LEU	C-N-CA	5.49	131.58	121.70
7	7	353	THR	CA-C-N	5.45	131.51	121.70
7	7	353	THR	C-N-CA	5.45	131.51	121.70
14	I	11	ARG	CA-C-N	5.43	131.75	121.97
14	I	11	ARG	C-N-CA	5.43	131.75	121.97
42	n	14	LYS	CA-C-N	5.41	131.88	121.54
42	n	14	LYS	C-N-CA	5.41	131.88	121.54
5	5	211	ILE	CA-C-N	5.41	128.93	120.82
5	5	211	ILE	C-N-CA	5.41	128.93	120.82
14	I	24	THR	N-CA-C	-5.39	106.64	113.43
10	A	141	A	P-O3'-C3'	5.36	128.23	120.20
36	h	94	PRO	CA-C-N	5.28	128.75	120.82
36	h	94	PRO	C-N-CA	5.28	128.75	120.82
3	3	75	THR	O-C-N	5.28	129.39	122.68
3	3	51	VAL	N-CA-C	5.27	120.30	109.34
10	A	317	G	P-O3'-C3'	5.25	128.08	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	417	GLN	N-CA-C	5.25	121.42	109.81
22	S	84	ASN	N-CA-C	5.25	116.74	110.44
43	o	9	HIS	CA-C-N	5.24	131.54	121.54
43	o	9	HIS	C-N-CA	5.24	131.54	121.54
2	2	603	PRO	N-CA-C	5.23	117.08	110.70
30	b	41	LYS	CA-C-N	5.23	131.39	121.97
30	b	41	LYS	C-N-CA	5.23	131.39	121.97
49	u	17	ILE	CB-CA-C	5.23	117.38	110.84
4	4	213	GLU	CA-C-N	5.22	128.47	122.83
4	4	213	GLU	C-N-CA	5.22	128.47	122.83
49	u	14	GLU	CA-C-N	5.21	131.22	123.05
49	u	14	GLU	C-N-CA	5.21	131.22	123.05
35	g	201	LYS	CA-C-N	5.19	134.46	121.80
35	g	201	LYS	C-N-CA	5.19	134.46	121.80
2	2	364	ASN	CA-C-N	5.18	131.44	121.54
2	2	364	ASN	C-N-CA	5.18	131.44	121.54
30	b	45	ARG	CA-C-N	5.17	129.01	121.31
30	b	45	ARG	C-N-CA	5.17	129.01	121.31
5	5	210	LEU	CA-C-N	5.14	131.22	121.97
5	5	210	LEU	C-N-CA	5.14	131.22	121.97
41	m	52	TYR	N-CA-C	-5.11	107.01	114.12
34	f	202	TYR	CA-C-N	5.11	131.30	121.54
34	f	202	TYR	C-N-CA	5.11	131.30	121.54
6	6	184	SER	N-CA-C	5.09	116.87	110.91
1	1	165	ARG	CA-C-N	5.08	131.25	121.54
1	1	165	ARG	C-N-CA	5.08	131.25	121.54
24	V	118	ASN	N-CA-C	5.07	118.91	112.12
2	2	418	ILE	CA-C-N	5.06	131.21	121.54
2	2	418	ILE	C-N-CA	5.06	131.21	121.54
41	m	278	SER	CA-C-N	5.06	130.81	121.70
41	m	278	SER	C-N-CA	5.06	130.81	121.70
6	6	151	GLN	CA-CB-CG	5.05	124.20	114.10
5	5	221	LYS	CA-C-N	5.03	131.15	121.54
5	5	221	LYS	C-N-CA	5.03	131.15	121.54
44	p	117	LEU	CA-C-N	5.02	131.13	121.54
44	p	117	LEU	C-N-CA	5.02	131.13	121.54
4	4	128	ARG	N-CA-C	-5.02	108.19	114.56
23	U	44	LYS	N-CA-C	-5.02	107.01	114.64
38	j	69	SER	CA-C-N	5.01	128.27	120.60
38	j	69	SER	C-N-CA	5.01	128.27	120.60
3	3	65	ASP	CA-C-N	5.01	124.34	120.33
3	3	65	ASP	C-N-CA	5.01	124.34	120.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	6	125	MET	CA-C-N	5.01	127.24	120.38
6	6	125	MET	C-N-CA	5.01	127.24	120.38

There are no chirality outliers.

All (132) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	264	LYS	Peptide
1	1	330	PRO	Peptide
1	1	384	VAL	Peptide
1	1	417	GLN	Peptide
1	1	485	ASP	Peptide
1	1	7	ARG	Peptide
2	2	386	ASN	Peptide
2	2	390	ALA	Peptide
2	2	415	ASN	Peptide
2	2	433	ASN	Peptide
2	2	552	CYS	Peptide
2	2	560	ARG	Peptide
2	2	603	PRO	Peptide
2	2	847	THR	Peptide
3	3	23	LEU	Peptide
3	3	237	LEU	Peptide
3	3	244	ASN	Peptide
3	3	245	ALA	Peptide
3	3	25	PHE	Peptide
3	3	250	CYS	Peptide
3	3	27	SER	Peptide
3	3	279	LYS	Peptide
3	3	324	PHE	Peptide
3	3	49	ASN	Peptide
3	3	50	MET	Peptide
3	3	91	ILE	Peptide
4	4	127	GLU	Peptide
4	4	128	ARG	Peptide
4	4	198	ASP	Peptide
4	4	214	ALA	Peptide
4	4	243	VAL	Peptide
4	4	284	GLY	Peptide
4	4	337	LYS	Peptide
4	4	338	ILE	Peptide
5	5	122	SER	Peptide

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Mol	Chain	Res	Type	Group
5	5	180	LYS	Peptide
5	5	221	LYS	Peptide
5	5	297	PRO	Peptide
7	7	252	ASP	Peptide
7	7	348	SER	Peptide
7	7	376	THR	Peptide
7	7	423	PRO	Peptide
8	8	106	LEU	Peptide
8	8	112	GLY	Peptide
8	8	115	LYS	Peptide
8	8	116	ASN	Peptide
8	8	117	THR	Peptide
8	8	218	PHE	Peptide
8	8	288	GLU	Peptide
8	8	335	SER	Peptide
9	9	376	ASN	Peptide
9	9	419	TRP	Peptide
9	9	426	GLN	Peptide
12	G	152	LYS	Peptide
13	H	41	MET	Peptide
13	H	43	GLU	Peptide
14	I	11	ARG	Peptide
14	I	168	LYS	Peptide
16	K	147	PHE	Peptide
17	L	15	VAL	Peptide
17	L	8	LYS	Peptide
17	L	94	LYS	Peptide
19	P	114	HIS	Peptide
19	P	117	GLU	Peptide
19	P	156	ALA	Peptide
19	P	165	SER	Peptide
19	P	170	GLU	Peptide
19	P	171	ASP	Peptide
19	P	172	GLU	Peptide
19	P	223	MET	Peptide
19	P	225	ILE	Peptide
19	P	47	LEU	Peptide
19	P	90	VAL	Peptide
22	S	85	GLU	Peptide
23	U	202	SER	Peptide
23	U	79	HIS	Peptide
24	V	118	ASN	Peptide

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Mol	Chain	Res	Type	Group
25	W	111	ARG	Peptide
25	W	112	ASN	Peptide
26	X	107	LYS	Peptide
26	X	16	PRO	Peptide
26	X	17	ASP	Peptide
26	X	189	PHE	Peptide
26	X	66	VAL	Peptide
27	Y	81	ARG	Peptide
30	b	40	ASP	Peptide
30	b	41	LYS	Peptide
31	c	161	LYS	Peptide
33	e	94	GLU	Peptide
34	f	202	TYR	Peptide
34	f	204	TYR	Peptide
34	f	207	PRO	Peptide
34	f	9	GLN	Peptide
35	g	202	LYS	Peptide
35	g	203	PRO	Peptide
36	h	46	LYS	Peptide
36	h	50	VAL	Peptide
37	i	105	LEU	Peptide
37	i	180	ASP	Peptide
37	i	208	HIS	Peptide
37	i	75	GLN	Peptide
37	i	76	ASN	Peptide
37	i	77	ASP	Peptide
38	j	127	GLY	Peptide
41	m	156	PHE	Peptide
41	m	59	LEU	Peptide
41	m	95	GLY	Peptide
42	n	125	PRO	Peptide
42	n	128	HIS	Peptide
42	n	15	PHE	Peptide
42	n	50	ARG	Peptide
43	o	10	LYS	Peptide
43	o	19	LYS	Peptide
44	p	104	LYS	Peptide
44	p	118	ARG	Peptide
44	p	135	HIS	Peptide
44	p	83	LYS	Peptide
44	p	90	LYS	Peptide
44	p	97	LYS	Peptide

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Mol	Chain	Res	Type	Group
45	q	151	ASP	Peptide
45	q	154	ARG	Peptide
45	q	67	VAL	Peptide
45	q	68	LEU	Peptide
46	r	118	SER	Peptide
46	r	30	GLY	Peptide
46	r	59	PRO	Peptide
46	r	93	LYS	Peptide
48	t	1	MET	Peptide
48	t	29	MET	Peptide
48	t	43	LEU	Peptide
49	u	8	LEU	Peptide
50	w	210	SER	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	1	4935	0	5017	236	0
2	2	4529	0	4533	161	0
3	3	3466	0	3446	122	0
4	4	2111	0	2105	117	0
5	5	2624	0	2592	105	0
6	6	1738	0	1706	84	0
7	7	3110	0	3084	103	0
8	8	2919	0	2950	136	0
9	9	2867	0	2838	113	0
10	A	37881	0	19144	0	0
11	F	544	0	283	0	0
12	G	1296	0	1374	0	0
13	H	1124	0	1193	0	0
14	I	2083	0	2189	0	0
15	J	445	0	442	0	0
16	K	1499	0	1608	0	0
17	L	1140	0	1191	0	0
18	N	1604	0	816	0	0
19	P	2147	0	2191	0	0
20	Q	1107	0	1179	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	R	1113	0	1149	0	0
22	S	3214	0	3354	0	0
23	U	1509	0	1563	0	0
24	V	473	0	524	0	0
25	W	599	0	656	0	0
26	X	1530	0	1627	0	0
27	Y	659	0	683	0	0
28	Z	1208	0	1294	0	0
29	a	1034	0	1080	0	0
30	b	620	0	622	0	0
31	c	1743	0	1836	0	0
32	d	147	0	146	0	0
33	e	1020	0	1075	0	0
34	f	1643	0	1646	0	0
35	g	1765	0	1863	0	0
36	h	822	0	887	0	0
37	i	1742	0	1815	0	0
38	j	1016	0	1039	0	0
39	k	790	0	839	0	0
40	l	507	0	536	0	0
41	m	2437	0	2393	0	0
42	n	1061	0	1120	0	0
43	o	1680	0	1762	0	0
44	p	582	0	599	0	0
45	q	1924	0	2089	0	0
46	r	958	0	993	0	0
47	s	1065	0	1137	0	0
48	t	828	0	854	0	0
49	u	608	0	598	17	0
50	w	3308	0	3236	62	0
51	1	1	0	0	0	0
51	9	376	0	0	28	0
51	A	6	0	0	1	0
51	H	5	0	0	0	0
51	U	13	0	0	1	0
51	j	1	0	0	0	0
51	l	8	0	0	0	0
51	m	5	0	0	0	0
All	All	117189	0	98896	1131	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 18.

All (1131) 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)
7:7:396:ASP:OD2	7:7:400:ARG:NH1	1.86	1.08
6:6:20:ARG:NH1	6:6:45:GLU:OE2	1.90	1.05
3:3:136:LYS:NZ	3:3:140:GLU:OE2	1.89	1.04
5:5:36:VAL:HG11	5:5:168:ARG:HH12	1.29	0.94
3:3:266:ASP:OD1	3:3:269:LYS:NZ	2.03	0.91
7:7:376:THR:O	7:7:461:ARG:NH1	2.07	0.88
1:1:169:ARG:HH11	1:1:173:LEU:HD22	1.38	0.88
1:1:454:ARG:HH11	8:8:327:GLN:HE21	1.19	0.87
2:2:441:ARG:NH1	2:2:491:GLU:OE2	2.06	0.87
1:1:402:LYS:HB3	1:1:406:ARG:HH12	1.38	0.86
8:8:79:GLN:OE1	8:8:115:LYS:NZ	2.08	0.86
1:1:483:ARG:NH1	1:1:493:PHE:O	2.09	0.84
49:u:68:ASN:OD1	49:u:69:ARG:NH1	2.10	0.84
7:7:239:ASN:OD1	7:7:242:ARG:NH1	2.11	0.83
3:3:13:PHE:O	3:3:16:ARG:NH1	2.12	0.83
8:8:51:VAL:O	8:8:89:LYS:NZ	2.11	0.83
9:9:345:ARG:NH1	51:9:601:HOH:O	2.11	0.82
2:2:781:ARG:NH1	2:2:784:GLN:OE1	2.13	0.82
9:9:464:ARG:NH1	9:9:467:VAL:O	2.13	0.82
1:1:500:ALA:HA	1:1:520:ARG:HH12	1.45	0.81
2:2:781:ARG:NH1	2:2:812:GLU:O	2.12	0.81
3:3:47:ASP:OD2	3:3:170:TRP:NE1	2.14	0.80
1:1:572:ARG:NH1	4:4:128:ARG:HH12	1.78	0.80
3:3:108:ARG:NH1	3:3:134:TYR:OH	2.13	0.80
8:8:54:LYS:O	8:8:89:LYS:NZ	2.17	0.78
1:1:321:ARG:NH1	1:1:421:GLU:OE2	2.17	0.78
1:1:579:LYS:NZ	5:5:71:VAL:O	2.15	0.77
3:3:74:ARG:NH1	3:3:140:GLU:O	2.18	0.77
1:1:402:LYS:O	1:1:406:ARG:NH1	2.17	0.77
9:9:444:LYS:NZ	51:9:607:HOH:O	2.17	0.77
3:3:229:ARG:NH1	3:3:230:ASP:OD1	2.17	0.76
2:2:476:GLU:OE2	2:2:509:HIS:ND1	2.16	0.76
50:w:361:ASP:OD2	50:w:404:ARG:NH1	2.19	0.76
9:9:296:GLU:OE2	9:9:321:ARG:NH1	2.19	0.76
2:2:611:ARG:NH1	2:2:675:LEU:O	2.19	0.75
9:9:233:ARG:NH1	9:9:336:GLN:OE1	2.19	0.75
1:1:572:ARG:HH11	4:4:128:ARG:NH1	1.85	0.75
9:9:520:LYS:NZ	9:9:521:ASP:O	2.19	0.74
2:2:733:MET:SD	2:2:760:LYS:NZ	2.58	0.74
2:2:515:ASP:OD2	2:2:622:ARG:NH2	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:394:LEU:O	1:1:438:ARG:NH1	2.22	0.73
1:1:445:GLN:NE2	1:1:503:GLU:OE2	2.19	0.72
4:4:373:LYS:HB3	7:7:544:ILE:HG13	1.71	0.72
6:6:186:GLN:HE21	7:7:508:ALA:H	1.35	0.72
2:2:484:GLU:OE2	2:2:506:ARG:NH1	2.23	0.72
1:1:463:ASP:OD2	1:1:466:GLN:N	2.16	0.72
1:1:300:TYR:OH	1:1:307:ARG:NH1	2.23	0.72
9:9:277:ASP:OD2	9:9:292:ARG:NH2	2.20	0.71
5:5:261:ASN:HB3	5:5:265:ARG:HH12	1.55	0.70
1:1:564:GLU:OE2	1:1:567:ARG:NH1	2.24	0.70
3:3:255:ARG:NH2	3:3:290:ASP:OD2	2.25	0.70
9:9:326:GLU:OE2	9:9:473:HIS:NE2	2.20	0.70
9:9:520:LYS:NZ	51:9:608:HOH:O	2.22	0.70
5:5:217:GLU:OE2	5:5:221:LYS:NZ	2.24	0.69
9:9:238:VAL:N	9:9:384:ARG:HH12	1.90	0.69
9:9:384:ARG:NH1	51:9:613:HOH:O	2.26	0.69
1:1:288:ASN:HD21	1:1:352:GLN:HG2	1.57	0.69
4:4:129:ARG:NH1	4:4:133:ALA:O	2.26	0.69
9:9:495:ASP:OD2	51:9:602:HOH:O	2.11	0.69
1:1:343:ASP:OD1	2:2:719:ARG:NH1	2.27	0.68
2:2:875:ASP:HA	5:5:276:GLN:HG3	1.75	0.68
1:1:169:ARG:NH1	1:1:173:LEU:HD22	2.08	0.68
9:9:238:VAL:H	9:9:384:ARG:HH12	1.40	0.68
3:3:9:ARG:HE	3:3:204:PRO:HD3	1.57	0.68
3:3:344:PHE:O	3:3:348:HIS:ND1	2.27	0.67
1:1:554:VAL:HG22	5:5:215:MET:HE3	1.76	0.67
1:1:572:ARG:HH11	4:4:128:ARG:HH12	1.39	0.67
6:6:48:LEU:HD13	6:6:84:LEU:HB3	1.77	0.67
8:8:23:LYS:HZ1	8:8:47:GLU:HG3	1.58	0.67
9:9:374:ASP:OD2	51:9:604:HOH:O	2.13	0.67
5:5:36:VAL:HG11	5:5:168:ARG:NH1	2.07	0.67
1:1:190:ARG:NH2	1:1:238:ASP:OD2	2.28	0.67
4:4:113:ARG:NE	4:4:150:GLU:OE2	2.18	0.67
9:9:211:GLU:OE2	51:9:603:HOH:O	2.13	0.67
8:8:336:HIS:O	8:8:344:LYS:NZ	2.27	0.67
9:9:371:ARG:NH1	51:9:615:HOH:O	2.28	0.67
1:1:495:SER:HB2	8:8:324:LYS:HD2	1.76	0.66
9:9:238:VAL:O	9:9:384:ARG:NH1	2.28	0.66
8:8:321:VAL:HG11	8:8:332:VAL:HB	1.78	0.66
3:3:27:SER:N	3:3:64:ASP:OD2	2.28	0.66
1:1:233:ARG:HE	1:1:279:VAL:HG21	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:9:369:ARG:HD3	9:9:371:ARG:HH11	1.59	0.66
4:4:126:TYR:HA	4:4:136:VAL:HG21	1.78	0.65
3:3:29:LYS:NZ	3:3:56:ASP:OD1	2.28	0.65
5:5:345:GLN:HE22	8:8:366:ASN:HD21	1.44	0.65
8:8:250:ALA:HB1	8:8:276:LYS:HG3	1.78	0.65
3:3:371:ILE:HA	3:3:374:LEU:HB2	1.78	0.65
50:w:484:HIS:HB2	50:w:491:SER:HB2	1.78	0.65
2:2:802:ILE:HB	2:2:842:VAL:HB	1.78	0.65
6:6:32:TYR:OH	6:6:43:ASP:OD2	2.10	0.65
3:3:124:ARG:HG3	3:3:155:ARG:HH12	1.62	0.65
9:9:276:TRP:H	9:9:520:LYS:HB3	1.62	0.65
1:1:99:GLU:CD	1:1:151:LYS:HZ3	2.04	0.65
1:1:107:GLU:OE2	1:1:187:GLN:NE2	2.30	0.65
2:2:619:CYS:HA	2:2:622:ARG:HB2	1.79	0.65
8:8:59:ASP:OD2	8:8:98:ARG:NH1	2.26	0.65
2:2:391:THR:HB	2:2:392:TYR:HB3	1.77	0.64
7:7:465:LYS:NZ	7:7:518:GLU:OE1	2.26	0.64
8:8:117:THR:HG23	8:8:120:ARG:HB2	1.79	0.64
7:7:262:ARG:NE	7:7:286:ASP:OD2	2.30	0.64
4:4:128:ARG:NH1	5:5:210:LEU:HD13	2.12	0.64
7:7:373:ILE:HA	7:7:398:MET:HG3	1.80	0.64
6:6:80:THR:HG22	7:7:327:ARG:HE	1.62	0.64
8:8:80:GLU:OE2	8:8:115:LYS:NZ	2.19	0.64
2:2:653:ARG:NH2	2:2:657:GLU:OE2	2.31	0.64
4:4:362:ASN:ND2	6:6:214:MET:SD	2.70	0.64
3:3:9:ARG:HH21	3:3:203:SER:HA	1.62	0.64
5:5:261:ASN:HB3	5:5:265:ARG:NH1	2.12	0.64
3:3:374:LEU:HB3	3:3:380:LEU:HB3	1.80	0.64
7:7:245:GLU:HA	7:7:439:PRO:HG2	1.79	0.64
1:1:14:ARG:HA	1:1:17:GLU:HB2	1.79	0.64
3:3:263:THR:HG21	3:3:331:ASP:HB3	1.80	0.63
8:8:80:GLU:HA	8:8:83:ILE:HG22	1.80	0.63
1:1:96:LEU:HD21	1:1:152:PHE:HB2	1.81	0.63
3:3:156:VAL:HG21	3:3:191:ARG:NH1	2.13	0.63
9:9:373:TRP:HB2	9:9:381:LEU:HB3	1.79	0.63
2:2:804:MET:HB2	2:2:840:GLN:HB3	1.81	0.63
6:6:15:LEU:HD13	6:6:45:GLU:HB3	1.79	0.62
9:9:312:ASP:OD2	51:9:605:HOH:O	2.15	0.62
2:2:578:LEU:HA	2:2:622:ARG:HH12	1.64	0.62
4:4:266:ARG:HA	4:4:269:VAL:HG12	1.82	0.62
9:9:375:LEU:HB2	9:9:379:ILE:HB	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:8:235:GLU:HG3	8:8:241:LEU:HD12	1.82	0.62
1:1:236:GLN:HE22	1:1:249:ALA:HB2	1.65	0.61
1:1:400:PRO:HD3	1:1:442:GLN:HE21	1.64	0.61
4:4:123:VAL:HA	4:4:126:TYR:HB3	1.80	0.61
9:9:262:ILE:HG23	9:9:278:ILE:HD13	1.82	0.61
8:8:321:VAL:HB	8:8:333:VAL:H	1.65	0.61
3:3:6:LEU:HG	3:3:9:ARG:HD3	1.82	0.61
1:1:58:CYS:HB3	1:1:62:ARG:NH1	2.16	0.61
8:8:242:THR:OG1	8:8:260:LYS:NZ	2.33	0.61
3:3:263:THR:HG22	3:3:335:ASN:HD22	1.65	0.61
1:1:159:GLN:HE22	1:1:169:ARG:HB3	1.66	0.61
50:w:349:LEU:HB2	50:w:365:LEU:HB2	1.81	0.61
1:1:200:ASN:O	1:1:204:HIS:N	2.34	0.61
1:1:221:ASN:ND2	1:1:224:GLU:OE1	2.33	0.61
8:8:90:LEU:HB3	8:8:99:PRO:HB3	1.81	0.61
1:1:189:THR:HB	1:1:192:ALA:HB3	1.83	0.60
1:1:572:ARG:HA	1:1:575:ILE:HB	1.82	0.60
50:w:341:PHE:HB3	50:w:352:TYR:HB2	1.82	0.60
9:9:343:GLU:OE2	51:9:606:HOH:O	2.16	0.60
8:8:197:ALA:O	8:8:201:ARG:NH1	2.33	0.60
8:8:285:MET:HG2	8:8:290:LYS:HA	1.84	0.60
2:2:748:ASP:OD2	2:2:751:THR:OG1	2.15	0.60
3:3:97:ASP:OD1	3:3:97:ASP:N	2.34	0.60
1:1:415:ARG:NH2	1:1:432:GLN:OE1	2.35	0.60
2:2:340:ARG:HG2	2:2:347:ARG:HH21	1.66	0.60
6:6:20:ARG:HD2	7:7:292:LYS:HZ3	1.67	0.60
7:7:476:ALA:HA	7:7:479:LEU:HB2	1.82	0.60
8:8:63:VAL:HG12	8:8:102:ARG:HE	1.66	0.60
6:6:48:LEU:HD22	6:6:84:LEU:HD13	1.84	0.60
1:1:216:THR:HG21	1:1:259:LEU:HD22	1.84	0.60
6:6:110:GLU:CD	7:7:327:ARG:HH12	2.09	0.60
9:9:477:GLU:OE2	9:9:479:GLN:NE2	2.35	0.60
50:w:388:GLU:OE1	50:w:414:ASN:ND2	2.35	0.60
7:7:329:TYR:OH	7:7:454:GLN:NE2	2.34	0.60
9:9:489:GLN:NE2	51:U:301:HOH:O	2.35	0.60
5:5:125:TYR:O	5:5:156:LYS:NZ	2.35	0.59
6:6:115:GLN:HE21	6:6:160:GLU:HG2	1.67	0.59
8:8:20:ALA:O	8:8:34:SER:OG	2.20	0.59
1:1:280:SER:O	1:1:284:TRP:N	2.35	0.59
4:4:116:PRO:O	4:4:120:ALA:N	2.35	0.59
9:9:256:VAL:HG22	9:9:287:LEU:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:554:VAL:O	1:1:558:LEU:N	2.36	0.59
6:6:87:CYS:HA	7:7:446:VAL:HG13	1.84	0.59
4:4:183:VAL:HA	5:5:85:PRO:HB3	1.85	0.59
49:u:8:LEU:HG	49:u:12:VAL:HG23	1.85	0.59
1:1:53:LYS:HA	1:1:91:ARG:HH12	1.68	0.59
8:8:74:LEU:HA	8:8:79:GLN:HA	1.85	0.59
9:9:180:VAL:HB	9:9:531:ASP:HB3	1.83	0.59
50:w:271:ILE:HG22	50:w:272:GLN:HG3	1.84	0.59
3:3:73:LYS:HB3	3:3:97:ASP:HB3	1.84	0.59
4:4:366:SER:OG	7:7:533:THR:O	2.21	0.59
7:7:223:ASN:HD22	7:7:352:ARG:NH1	2.01	0.59
6:6:20:ARG:HH12	7:7:295:GLU:CD	2.11	0.58
1:1:496:ASP:OD1	4:4:337:LYS:NZ	2.35	0.58
2:2:329:VAL:HG13	2:2:357:LEU:HD22	1.84	0.58
4:4:223:ASP:HB2	4:4:234:LYS:HE2	1.84	0.58
1:1:77:ILE:HG12	1:1:84:LYS:HZ2	1.67	0.58
1:1:90:VAL:HG22	1:1:172:ARG:HH12	1.68	0.58
4:4:109:GLY:O	8:8:104:GLN:NE2	2.36	0.58
4:4:123:VAL:O	4:4:127:GLU:N	2.36	0.58
8:8:221:ASP:OD1	8:8:339:HIS:ND1	2.33	0.58
9:9:246:ILE:HD11	9:9:384:ARG:HB2	1.84	0.58
6:6:151:GLN:HB2	7:7:505:GLY:HA3	1.86	0.58
1:1:173:LEU:HA	1:1:176:ASP:HB2	1.84	0.58
4:4:113:ARG:HD2	4:4:260:ALA:HB3	1.84	0.58
8:8:186:VAL:HA	8:8:189:LEU:HB3	1.86	0.58
1:1:323:LEU:HB3	1:1:383:VAL:HG13	1.86	0.58
3:3:46:SER:OG	3:3:49:ASN:ND2	2.37	0.58
4:4:317:LYS:HZ2	4:4:321:ASP:HA	1.68	0.58
1:1:181:ALA:HB1	1:1:196:LYS:HZ1	1.69	0.58
3:3:383:LYS:HA	7:7:466:LEU:HD22	1.85	0.58
8:8:320:MET:SD	8:8:338:THR:OG1	2.60	0.58
9:9:421:ARG:NH2	51:A:1903:HOH:O	2.36	0.58
9:9:506:ASP:O	9:9:510:ASN:ND2	2.37	0.58
8:8:197:ALA:HB1	8:8:201:ARG:HH12	1.68	0.57
3:3:108:ARG:NH1	3:3:134:TYR:HH	2.01	0.57
4:4:336:PRO:HB3	5:5:350:TYR:HA	1.84	0.57
8:8:23:LYS:HZ1	8:8:47:GLU:CG	2.17	0.57
6:6:36:GLN:NE2	6:6:43:ASP:O	2.38	0.57
6:6:43:ASP:O	6:6:47:ASN:ND2	2.37	0.57
6:6:214:MET:HA	7:7:534:LYS:NZ	2.20	0.57
49:u:10:TYR:OH	49:u:39:GLU:OE2	2.21	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:650:LEU:HB2	2:2:653:ARG:HB2	1.87	0.57
1:1:395:GLU:HA	1:1:438:ARG:HH12	1.69	0.57
1:1:402:LYS:HB3	1:1:406:ARG:NH1	2.15	0.57
4:4:304:SER:O	8:8:348:GLN:NE2	2.37	0.57
50:w:261:ALA:HA	50:w:273:ARG:HA	1.85	0.57
2:2:374:ILE:O	2:2:378:ILE:N	2.37	0.57
3:3:229:ARG:HA	3:3:232:ILE:HG22	1.87	0.57
5:5:53:TYR:O	5:5:64:GLN:NE2	2.38	0.57
8:8:367:SER:HA	8:8:370:SER:HB2	1.86	0.57
50:w:451:ARG:HH12	50:w:501:GLY:HA2	1.69	0.57
1:1:485:ASP:HB3	2:2:803:SER:H	1.69	0.57
5:5:154:PRO:HD2	5:5:156:LYS:HE3	1.87	0.57
50:w:309:ILE:HG21	50:w:357:MET:HE3	1.87	0.57
50:w:447:PHE:HB2	50:w:463:GLU:HB3	1.87	0.57
3:3:4:TYR:OH	3:3:211:ARG:NH2	2.37	0.57
5:5:185:GLU:HB3	5:5:189:LYS:HE3	1.87	0.57
3:3:50:MET:HB2	3:3:178:LEU:HD22	1.87	0.56
50:w:247:PRO:HG3	50:w:286:PRO:HA	1.87	0.56
1:1:271:LEU:HD13	1:1:306:MET:HG3	1.86	0.56
1:1:587:ILE:HG22	1:1:591:LYS:NZ	2.20	0.56
1:1:198:CYS:HB3	1:1:202:ARG:HH12	1.70	0.56
1:1:395:GLU:O	1:1:512:GLN:NE2	2.38	0.56
3:3:77:VAL:HG13	3:3:97:ASP:HB2	1.87	0.56
4:4:286:SER:OG	5:5:159:GLN:O	2.23	0.56
7:7:242:ARG:O	7:7:427:ASN:ND2	2.34	0.56
9:9:389:ALA:HB3	9:9:401:LEU:HB2	1.87	0.56
1:1:13:LYS:HZ1	1:1:39:LYS:HZ2	1.53	0.56
2:2:591:MET:HB3	3:3:11:ALA:HB2	1.88	0.56
3:3:125:GLN:O	3:3:129:ASP:N	2.36	0.56
6:6:20:ARG:NH1	7:7:295:GLU:OE2	2.39	0.56
6:6:23:PRO:HA	6:6:53:LEU:HD13	1.87	0.56
9:9:458:LYS:NZ	9:9:480:GLN:HB2	2.21	0.56
8:8:254:LYS:O	8:8:258:ASN:ND2	2.39	0.56
1:1:521:ASN:HB3	5:5:245:LEU:HB3	1.86	0.56
3:3:39:GLN:NE2	3:3:52:ASP:O	2.38	0.56
1:1:442:GLN:HE22	1:1:514:MET:HG3	1.69	0.56
2:2:386:ASN:HD22	2:2:393:MET:HG3	1.71	0.56
8:8:127:LEU:HA	8:8:130:VAL:HB	1.88	0.56
8:8:167:LEU:O	8:8:171:ALA:N	2.38	0.56
8:8:297:MET:HA	8:8:300:GLU:HB2	1.88	0.56
2:2:769:PHE:HB2	2:2:772:ALA:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:w:470:ALA:HB3	50:w:483:LEU:HB2	1.87	0.56
1:1:141:THR:O	1:1:145:LEU:N	2.32	0.56
3:3:380:LEU:HD11	3:3:393:MET:HG3	1.88	0.56
7:7:241:ASN:HB2	7:7:289:GLN:HE22	1.71	0.56
1:1:95:LYS:HB3	1:1:151:LYS:HB3	1.88	0.56
8:8:23:LYS:NZ	8:8:50:ASP:HB2	2.21	0.56
8:8:118:PRO:HA	8:8:121:TYR:HB3	1.87	0.56
3:3:350:CYS:SG	3:3:351:ILE:N	2.79	0.55
7:7:363:GLN:NE2	7:7:419:LYS:O	2.39	0.55
5:5:274:LYS:HB3	5:5:308:PRO:HB2	1.88	0.55
5:5:336:GLN:HB3	5:5:340:LYS:NZ	2.22	0.55
49:u:31:LEU:HD13	49:u:33:ARG:HB3	1.88	0.55
4:4:369:ALA:HA	4:4:372:GLU:HB3	1.88	0.55
8:8:45:ILE:O	8:8:49:CYS:N	2.40	0.55
1:1:314:GLU:HB2	1:1:318:MET:HG3	1.88	0.55
2:2:340:ARG:NH1	2:2:384:ASP:OD2	2.39	0.55
4:4:181:LYS:HD3	4:4:185:PRO:HA	1.89	0.55
7:7:236:ASP:OD2	7:7:262:ARG:NH1	2.38	0.55
1:1:557:TYR:O	1:1:561:SER:N	2.40	0.55
2:2:588:LEU:HA	2:2:591:MET:HB2	1.88	0.55
4:4:349:SER:O	4:4:353:ASP:N	2.40	0.55
1:1:266:PRO:HB2	1:1:269:PRO:HD2	1.86	0.55
2:2:333:LEU:HD11	2:2:377:ASN:HD22	1.71	0.55
3:3:70:LEU:HB3	3:3:71:ARG:HH11	1.72	0.55
1:1:13:LYS:HZ3	1:1:35:MET:HE3	1.72	0.55
1:1:558:LEU:HA	1:1:561:SER:HB3	1.88	0.55
2:2:867:VAL:HA	2:2:870:ASN:HB2	1.89	0.55
3:3:225:HIS:O	3:3:229:ARG:N	2.38	0.55
7:7:241:ASN:HA	7:7:244:LEU:HB3	1.89	0.55
8:8:161:LYS:O	8:8:165:LEU:N	2.37	0.55
50:w:487:ALA:O	50:w:491:SER:OG	2.23	0.55
1:1:267:PRO:O	1:1:271:LEU:N	2.39	0.54
1:1:454:ARG:NH1	8:8:327:GLN:HE21	1.98	0.54
2:2:666:GLU:OE1	2:2:669:ARG:NH2	2.40	0.54
9:9:444:LYS:NZ	51:9:669:HOH:O	2.38	0.54
1:1:283:PHE:O	1:1:287:GLY:N	2.40	0.54
5:5:171:PRO:HA	5:5:174:MET:HB2	1.89	0.54
8:8:20:ALA:HB2	8:8:47:GLU:OE2	2.07	0.54
2:2:398:TRP:NE1	2:2:451:MET:O	2.32	0.54
2:2:678:ASN:ND2	2:2:680:GLU:OE1	2.41	0.54
4:4:114:LEU:HD23	4:4:151:VAL:HB	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:171:LYS:HA	6:6:174:MET:HB3	1.88	0.54
7:7:376:THR:HB	7:7:402:GLN:HE22	1.73	0.54
8:8:108:ASN:HD21	8:8:142:THR:HG22	1.73	0.54
49:u:41:LEU:HD12	49:u:69:ARG:NH1	2.22	0.54
1:1:568:ILE:HG23	1:1:572:ARG:HB3	1.89	0.54
3:3:188:ASP:HA	3:3:191:ARG:HB2	1.89	0.54
3:3:371:ILE:HG21	3:3:391:VAL:HG11	1.89	0.54
5:5:66:VAL:HA	5:5:119:TRP:HA	1.90	0.54
6:6:182:ASP:HB3	6:6:186:GLN:HB2	1.88	0.54
7:7:240:ILE:HG23	7:7:253:PRO:HB2	1.88	0.54
1:1:561:SER:O	1:1:565:HIS:N	2.36	0.54
4:4:375:VAL:O	5:5:313:ARG:NH1	2.40	0.54
5:5:36:VAL:HA	5:5:146:GLU:HG3	1.89	0.54
3:3:376:ARG:NH1	7:7:481:LEU:HG	2.22	0.54
1:1:102:GLU:HB3	1:1:144:LEU:HD13	1.90	0.54
1:1:106:GLU:HA	1:1:109:GLN:HB2	1.90	0.54
1:1:348:ILE:HG23	2:2:725:PRO:HB3	1.90	0.54
2:2:515:ASP:O	2:2:519:HIS:ND1	2.33	0.54
5:5:44:LEU:HD13	5:5:210:LEU:HG	1.89	0.54
8:8:66:SER:O	8:8:70:LEU:N	2.40	0.54
9:9:523:ASN:ND2	51:9:635:HOH:O	2.41	0.54
1:1:317:ARG:O	1:1:321:ARG:N	2.41	0.54
5:5:69:GLY:HA2	5:5:78:ILE:HA	1.89	0.54
8:8:246:SER:OG	8:8:258:ASN:ND2	2.35	0.54
8:8:314:ASP:OD1	8:8:317:ARG:NH2	2.40	0.54
1:1:551:GLN:HA	5:5:219:GLU:HB2	1.90	0.54
49:u:9:PRO:HB3	49:u:69:ARG:HB2	1.90	0.54
4:4:135:ARG:NH2	4:4:161:GLU:OE1	2.41	0.54
9:9:329:PHE:O	9:9:333:ASN:ND2	2.40	0.54
50:w:368:SER:HB3	50:w:390:LYS:HG3	1.89	0.54
50:w:429:LEU:HB3	50:w:450:PHE:HB2	1.90	0.54
1:1:585:LEU:O	1:1:589:ARG:N	2.42	0.53
4:4:317:LYS:NZ	4:4:321:ASP:HA	2.21	0.53
7:7:421:LEU:HB3	7:7:443:GLN:HG2	1.89	0.53
4:4:360:LEU:HA	4:4:363:LEU:HD12	1.90	0.53
6:6:45:GLU:HA	6:6:48:LEU:HB3	1.90	0.53
2:2:459:MET:SD	2:2:674:HIS:NE2	2.81	0.53
2:2:766:TRP:HE1	2:2:776:ARG:HB2	1.73	0.53
9:9:426:GLN:HB3	9:9:429:ALA:HB3	1.91	0.53
4:4:243:VAL:HG11	4:4:248:MET:HA	1.89	0.53
5:5:176:VAL:HB	5:5:189:LYS:HE2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:w:262:LEU:HB2	50:w:272:GLN:HB2	1.91	0.53
50:w:597:ASN:HB3	50:w:599:LYS:NZ	2.24	0.53
1:1:554:VAL:HG13	5:5:215:MET:HG3	1.89	0.53
2:2:438:LEU:O	2:2:442:GLY:N	2.39	0.53
2:2:753:HIS:HE1	2:2:780:VAL:HA	1.71	0.53
6:6:47:ASN:HB3	6:6:69:ILE:HG23	1.90	0.53
6:6:67:ALA:HA	6:6:70:LEU:HB2	1.90	0.53
9:9:369:ARG:N	9:9:385:CYS:O	2.39	0.53
1:1:170:VAL:HG21	1:1:220:LEU:HG	1.91	0.53
2:2:517:LYS:O	2:2:521:ARG:N	2.41	0.53
2:2:591:MET:HG2	3:3:7:THR:HB	1.90	0.53
5:5:79:THR:HG21	5:5:112:ILE:HG13	1.90	0.53
7:7:504:SER:HA	7:7:515:SER:HA	1.90	0.53
8:8:120:ARG:O	8:8:124:TYR:N	2.37	0.53
1:1:122:GLN:O	1:1:126:SER:N	2.40	0.53
1:1:579:LYS:HG3	5:5:70:LEU:HD22	1.90	0.53
5:5:329:ASN:CG	7:7:537:ARG:HH12	2.17	0.53
9:9:303:ASN:ND2	51:9:651:HOH:O	2.42	0.53
50:w:555:TYR:H	50:w:596:LYS:HZ1	1.56	0.53
1:1:396:VAL:HA	1:1:512:GLN:HE22	1.73	0.53
1:1:450:ILE:HG12	1:1:455:LEU:HD13	1.91	0.53
3:3:185:ALA:O	3:3:189:LEU:N	2.39	0.53
4:4:179:LEU:HB3	5:5:103:MET:HE2	1.91	0.53
7:7:284:LEU:HA	7:7:287:TYR:HB3	1.91	0.53
8:8:74:LEU:HD22	8:8:79:GLN:HG3	1.90	0.53
9:9:211:GLU:HG3	9:9:345:ARG:HG2	1.91	0.53
9:9:226:LYS:O	9:9:475:ILE:N	2.36	0.53
9:9:239:THR:HB	9:9:291:LYS:HG3	1.91	0.53
9:9:316:SER:O	9:9:322:ASN:ND2	2.38	0.53
1:1:53:LYS:HG3	1:1:84:LYS:HE2	1.91	0.53
1:1:58:CYS:HB3	1:1:62:ARG:HH12	1.74	0.53
1:1:235:VAL:HG12	1:1:240:ALA:HB2	1.91	0.53
4:4:112:VAL:HA	4:4:149:VAL:HB	1.91	0.53
4:4:125:SER:HA	5:5:111:ASN:HD21	1.74	0.53
4:4:290:GLN:HB3	8:8:366:ASN:HB3	1.90	0.53
9:9:403:ILE:HG12	9:9:458:LYS:HB2	1.89	0.53
9:9:438:ASN:ND2	51:9:651:HOH:O	2.42	0.53
9:9:438:ASN:ND2	51:9:686:HOH:O	2.42	0.53
1:1:9:GLU:O	1:1:13:LYS:N	2.42	0.53
1:1:32:TYR:HB3	1:1:36:LYS:HE3	1.91	0.53
1:1:562:ARG:HG2	4:4:226:LEU:HD11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:563:ARG:HA	2:2:601:ALA:HB1	1.90	0.53
3:3:108:ARG:O	3:3:112:MET:N	2.41	0.53
50:w:391:ASP:N	50:w:391:ASP:OD1	2.41	0.53
1:1:454:ARG:HH11	8:8:327:GLN:NE2	1.98	0.52
3:3:145:SER:OG	3:3:179:MET:SD	2.67	0.52
3:3:312:LEU:O	3:3:316:GLU:N	2.39	0.52
9:9:208:GLY:HA3	9:9:367:ALA:HA	1.91	0.52
2:2:419:PHE:HA	2:2:429:GLU:HA	1.92	0.52
2:2:549:GLU:HB2	2:2:572:HIS:CD2	2.43	0.52
7:7:248:THR:OG1	7:7:249:SER:N	2.43	0.52
1:1:502:ARG:HH12	2:2:849:PRO:CB	2.21	0.52
2:2:498:GLU:O	2:2:502:VAL:N	2.34	0.52
3:3:229:ARG:O	3:3:233:ILE:N	2.41	0.52
6:6:68:GLN:HG3	6:6:127:LEU:HD21	1.92	0.52
8:8:23:LYS:NZ	8:8:47:GLU:O	2.41	0.52
50:w:209:TYR:HB3	50:w:608:ARG:HB3	1.90	0.52
1:1:29:ASP:HA	1:1:32:TYR:HD2	1.73	0.52
1:1:70:GLY:HA2	1:1:73:GLN:HB2	1.90	0.52
2:2:357:LEU:HA	2:2:360:ILE:HG22	1.90	0.52
3:3:221:VAL:HB	3:3:327:ALA:HB3	1.91	0.52
7:7:258:GLY:HA2	7:7:262:ARG:HB2	1.91	0.52
1:1:53:LYS:O	1:1:91:ARG:NH2	2.39	0.52
3:3:38:LEU:HD13	3:3:251:PRO:HG2	1.91	0.52
6:6:11:VAL:HG22	6:6:29:LEU:HD23	1.91	0.52
7:7:229:ASN:ND2	7:7:275:VAL:O	2.42	0.52
9:9:398:THR:N	51:9:693:HOH:O	2.42	0.52
49:u:40:ARG:HH12	49:u:42:LYS:HG3	1.75	0.52
1:1:340:ARG:HB2	2:2:722:GLU:OE2	2.09	0.52
1:1:395:GLU:HA	1:1:438:ARG:NH1	2.25	0.52
5:5:275:HIS:CE1	5:5:313:ARG:H	2.27	0.52
9:9:391:MET:O	9:9:399:GLN:N	2.41	0.52
9:9:490:ILE:HG13	9:9:491:ASN:H	1.74	0.52
9:9:493:ASN:ND2	51:9:697:HOH:O	2.43	0.52
3:3:49:ASN:O	3:3:53:PHE:N	2.43	0.52
3:3:168:SER:O	3:3:172:LYS:N	2.38	0.52
3:3:211:ARG:HD3	3:3:242:TYR:HB3	1.92	0.52
4:4:251:MET:HE1	8:8:68:VAL:HG22	1.92	0.52
6:6:16:LYS:NZ	7:7:295:GLU:HG2	2.25	0.52
9:9:384:ARG:NH2	51:9:694:HOH:O	2.42	0.52
9:9:523:ASN:ND2	51:9:698:HOH:O	2.43	0.52
4:4:266:ARG:NH1	5:5:231:LEU:HD23	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:130:THR:O	5:5:134:LEU:N	2.42	0.52
9:9:338:VAL:HG21	9:9:403:ILE:HG21	1.92	0.52
1:1:530:LEU:HG	5:5:234:ALA:HA	1.91	0.52
2:2:482:ILE:HA	2:2:485:ARG:HB2	1.92	0.52
2:2:595:GLN:OE1	2:2:609:TYR:OH	2.27	0.52
3:3:84:LEU:HD13	3:3:91:ILE:HG12	1.92	0.52
7:7:296:ASN:HD21	7:7:319:VAL:HG22	1.74	0.52
9:9:244:PRO:O	9:9:248:LYS:N	2.43	0.52
8:8:348:GLN:NE2	8:8:352:ASP:OD2	2.43	0.52
49:u:58:ALA:HB1	49:u:73:VAL:HG21	1.91	0.52
1:1:155:GLU:HB3	1:1:173:LEU:HD21	1.91	0.51
1:1:163:LEU:HD13	1:1:212:HIS:HB2	1.92	0.51
2:2:805:GLU:OE2	2:2:840:GLN:HB2	2.10	0.51
4:4:159:HIS:HE1	4:4:168:VAL:HG13	1.75	0.51
1:1:314:GLU:H	1:1:318:MET:HE2	1.76	0.51
1:1:414:VAL:O	1:1:425:GLN:NE2	2.42	0.51
3:3:70:LEU:HB3	3:3:71:ARG:NH1	2.25	0.51
4:4:272:ILE:O	4:4:276:CYS:N	2.34	0.51
4:4:354:LEU:HD22	5:5:246:LEU:HD23	1.92	0.51
6:6:91:GLN:NE2	6:6:95:GLU:OE2	2.43	0.51
8:8:346:GLN:O	8:8:350:LEU:N	2.43	0.51
9:9:420:ARG:NH2	9:9:464:ARG:O	2.42	0.51
1:1:148:PRO:O	1:1:152:PHE:N	2.40	0.51
1:1:230:LEU:HD23	1:1:233:ARG:HD3	1.92	0.51
2:2:815:LEU:HA	2:2:818:VAL:HB	1.91	0.51
2:2:834:SER:N	2:2:843:VAL:O	2.42	0.51
3:3:416:GLN:HG3	3:3:420:MET:HE3	1.91	0.51
9:9:211:GLU:HB2	9:9:339:LEU:HD22	1.92	0.51
50:w:249:GLY:O	50:w:608:ARG:NH2	2.43	0.51
2:2:395:PRO:HA	2:2:398:TRP:HB3	1.92	0.51
2:2:695:ILE:HA	2:2:698:MET:HG2	1.92	0.51
3:3:91:ILE:O	3:3:93:LYS:N	2.44	0.51
3:3:174:ALA:O	3:3:178:LEU:N	2.41	0.51
3:3:239:GLN:OE1	3:3:282:GLN:NE2	2.43	0.51
4:4:207:HIS:O	4:4:211:SER:N	2.41	0.51
7:7:265:LEU:HA	7:7:268:MET:HE2	1.92	0.51
1:1:108:SER:O	1:1:112:VAL:N	2.41	0.51
2:2:460:GLN:NE2	2:2:667:ARG:O	2.44	0.51
7:7:373:ILE:O	7:7:402:GLN:NE2	2.42	0.51
1:1:13:LYS:NZ	1:1:39:LYS:NZ	2.59	0.51
2:2:406:ASN:OD1	2:2:485:ARG:NH1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:836:ASP:O	2:2:840:GLN:N	2.43	0.51
3:3:49:ASN:HA	3:3:50:MET:HB2	1.93	0.51
4:4:324:VAL:HA	4:4:327:PHE:HB2	1.92	0.51
9:9:384:ARG:NH2	51:9:655:HOH:O	2.41	0.51
50:w:410:ARG:NH2	50:w:448:GLU:OE1	2.44	0.51
1:1:354:ARG:O	1:1:357:THR:OG1	2.23	0.51
2:2:329:VAL:O	2:2:333:LEU:N	2.43	0.51
2:2:568:ALA:O	2:2:572:HIS:N	2.40	0.51
4:4:141:LEU:HB3	4:4:187:GLU:HB3	1.92	0.51
4:4:195:THR:HA	4:4:222:VAL:HB	1.93	0.51
7:7:246:VAL:HA	7:7:435:TYR:HB3	1.93	0.51
8:8:301:LEU:HD13	8:8:311:PHE:HD2	1.75	0.51
1:1:222:ASN:O	1:1:225:SER:OG	2.23	0.51
1:1:580:GLU:HA	5:5:113:ASP:HB2	1.93	0.51
2:2:506:ARG:O	2:2:510:THR:OG1	2.26	0.51
4:4:263:ASP:OD2	5:5:235:SER:OG	2.16	0.51
6:6:113:HIS:HB3	6:6:116:ALA:HB3	1.93	0.51
2:2:633:LEU:HB3	2:2:637:GLN:HB2	1.93	0.51
3:3:35:LYS:NZ	3:3:322:ASP:HA	2.25	0.51
3:3:393:MET:HE2	3:3:395:ASN:HD22	1.76	0.51
8:8:281:THR:HG23	8:8:332:VAL:HG11	1.92	0.51
9:9:303:ASN:ND2	51:9:642:HOH:O	2.43	0.51
2:2:501:ARG:O	2:2:505:ARG:N	2.42	0.50
6:6:110:GLU:OE1	7:7:327:ARG:NH1	2.44	0.50
6:6:121:LEU:HD11	6:6:128:LEU:HD11	1.93	0.50
9:9:419:TRP:HE3	9:9:476:LEU:HD12	1.75	0.50
1:1:295:THR:O	1:1:299:LEU:N	2.40	0.50
3:3:35:LYS:HZ3	3:3:322:ASP:HA	1.76	0.50
3:3:128:LEU:HD23	3:3:131:LEU:HD23	1.93	0.50
1:1:172:ARG:HB3	1:1:176:ASP:OD2	2.11	0.50
1:1:294:SER:HA	1:1:361:LEU:HD23	1.93	0.50
2:2:418:ILE:HG23	2:2:429:GLU:OE2	2.10	0.50
2:2:516:TYR:OH	2:2:768:LEU:O	2.29	0.50
2:2:540:GLU:O	2:2:544:SER:N	2.44	0.50
6:6:19:ASP:O	6:6:25:ASN:ND2	2.43	0.50
8:8:23:LYS:HE3	8:8:34:SER:HA	1.93	0.50
4:4:319:SER:O	4:4:323:THR:OG1	2.26	0.50
9:9:233:ARG:HD3	9:9:364:ALA:HA	1.93	0.50
1:1:44:GLN:HA	1:1:48:GLU:HB2	1.94	0.50
1:1:169:ARG:HA	1:1:173:LEU:H	1.76	0.50
4:4:172:PHE:HA	4:4:175:ASN:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:8:23:LYS:HZ3	8:8:50:ASP:HB2	1.77	0.50
49:u:12:VAL:HG11	49:u:33:ARG:HH11	1.77	0.50
1:1:172:ARG:O	1:1:176:ASP:N	2.39	0.50
2:2:383:TYR:HA	2:2:393:MET:HE1	1.93	0.50
2:2:495:THR:HA	2:2:502:VAL:HG11	1.94	0.50
3:3:204:PRO:HA	3:3:207:SER:HB2	1.93	0.50
7:7:262:ARG:HB3	7:7:283:LEU:HD23	1.93	0.50
9:9:172:SER:N	51:9:702:HOH:O	2.44	0.50
50:w:223:TRP:N	50:w:230:VAL:O	2.41	0.50
1:1:375:VAL:HG22	1:1:380:LEU:HD22	1.92	0.50
2:2:548:MET:HA	2:2:551:LEU:HB3	1.94	0.50
3:3:304:ASP:HB3	3:3:308:ALA:HB2	1.94	0.50
4:4:287:SER:HB3	8:8:370:SER:HA	1.94	0.50
8:8:157:THR:HG22	8:8:161:LYS:HE2	1.94	0.50
50:w:215:SER:O	50:w:218:ARG:NH2	2.45	0.50
2:2:587:ASP:O	2:2:591:MET:N	2.44	0.50
3:3:315:CYS:O	3:3:319:LEU:N	2.43	0.50
5:5:50:ILE:HA	5:5:53:TYR:HB3	1.94	0.50
5:5:274:LYS:HG3	5:5:310:PRO:HD2	1.94	0.50
9:9:300:LEU:HB3	9:9:441:LYS:HD2	1.94	0.50
4:4:306:VAL:O	4:4:310:ALA:N	2.44	0.49
5:5:104:MET:HB2	5:5:114:HIS:HB2	1.93	0.49
8:8:277:MET:HA	8:8:301:LEU:HD21	1.93	0.49
9:9:260:ASP:OD2	9:9:386:GLU:HG2	2.11	0.49
9:9:281:GLU:HA	9:9:515:LYS:HA	1.94	0.49
9:9:371:ARG:NH1	51:9:610:HOH:O	2.25	0.49
9:9:512:LYS:O	9:9:516:TYR:OH	2.23	0.49
4:4:157:VAL:HG21	4:4:173:ALA:HB2	1.94	0.49
7:7:383:ASP:HA	7:7:391:ARG:HD2	1.94	0.49
8:8:312:VAL:HG21	8:8:331:LYS:HE3	1.93	0.49
1:1:454:ARG:NH1	8:8:327:GLN:HG3	2.27	0.49
3:3:388:LEU:HB3	3:3:390:HIS:HD2	1.77	0.49
4:4:323:THR:O	4:4:327:PHE:N	2.41	0.49
6:6:210:VAL:HG13	7:7:530:ILE:HG21	1.94	0.49
7:7:497:MET:SD	7:7:504:SER:OG	2.63	0.49
8:8:47:GLU:HA	8:8:50:ASP:OD2	2.13	0.49
1:1:441:GLN:HB3	1:1:511:LEU:HD22	1.92	0.49
1:1:489:ARG:NE	2:2:806:THR:OG1	2.42	0.49
2:2:834:SER:OG	3:3:396:ASN:OD1	2.26	0.49
3:3:124:ARG:HG3	3:3:155:ARG:NH1	2.26	0.49
1:1:93:TYR:HA	1:1:180:GLN:HE21	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:211:ARG:HH12	3:3:236:PHE:HB3	1.77	0.49
4:4:174:LYS:O	4:4:178:GLU:N	2.44	0.49
5:5:134:LEU:HD11	5:5:169:LEU:HD13	1.94	0.49
9:9:458:LYS:HZ2	9:9:480:GLN:HB2	1.77	0.49
2:2:391:THR:H	2:2:392:TYR:C	2.21	0.49
2:2:557:ALA:HB2	3:3:12:HIS:HB3	1.93	0.49
3:3:111:ARG:HE	3:3:133:ARG:HG2	1.78	0.49
4:4:269:VAL:HA	4:4:272:ILE:HB	1.93	0.49
6:6:214:MET:HA	7:7:534:LYS:HZ1	1.76	0.49
7:7:331:ASP:HA	7:7:334:ARG:HH21	1.77	0.49
8:8:282:PHE:HZ	8:8:340:ARG:HB2	1.78	0.49
4:4:375:VAL:HG11	5:5:318:LEU:HD11	1.95	0.49
5:5:190:ALA:HB2	5:5:315:ASP:OD2	2.12	0.49
8:8:201:ARG:HA	8:8:238:HIS:CD2	2.48	0.49
9:9:388:ASP:OD2	9:9:403:ILE:N	2.36	0.49
2:2:420:VAL:HG22	2:2:431:LEU:HD12	1.95	0.49
2:2:694:GLU:HA	2:2:697:TYR:HB3	1.95	0.49
2:2:789:ARG:NH2	2:2:821:ILE:O	2.45	0.49
4:4:152:THR:OG1	4:4:187:GLU:OE2	2.16	0.49
1:1:390:LEU:HD13	1:1:410:VAL:HB	1.95	0.49
6:6:151:GLN:HE21	6:6:195:SER:HB2	1.77	0.49
7:7:240:ILE:HG13	7:7:257:ALA:HB2	1.94	0.49
9:9:259:THR:HA	9:9:384:ARG:HB3	1.95	0.49
1:1:89:VAL:HG22	1:1:169:ARG:NH1	2.28	0.49
2:2:340:ARG:HA	2:2:345:THR:HG21	1.93	0.49
3:3:152:TYR:HD1	3:3:156:VAL:HG13	1.78	0.49
4:4:170:MET:O	4:4:174:LYS:N	2.45	0.49
9:9:379:ILE:HG21	9:9:505:ILE:HD13	1.95	0.49
3:3:135:ALA:HB2	3:3:158:VAL:HB	1.95	0.48
4:4:137:ILE:HA	4:4:194:ALA:HA	1.94	0.48
6:6:195:SER:OG	7:7:503:THR:O	2.29	0.48
8:8:114:ASP:HA	8:8:119:VAL:HB	1.94	0.48
1:1:101:THR:HA	1:1:104:ALA:HB3	1.95	0.48
1:1:199:ASP:HB3	1:1:203:MET:HE2	1.95	0.48
1:1:267:PRO:HA	1:1:270:GLN:HB2	1.94	0.48
3:3:207:SER:O	3:3:211:ARG:N	2.40	0.48
5:5:87:HIS:HB2	5:5:93:ASP:HB2	1.94	0.48
7:7:471:PRO:O	7:7:475:LEU:N	2.38	0.48
49:u:29:VAL:HG22	49:u:48:GLU:H	1.78	0.48
2:2:516:TYR:CZ	2:2:770:PRO:HD3	2.48	0.48
5:5:150:LEU:HA	5:5:166:ALA:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:488:ILE:HB	7:7:492:VAL:HG23	1.95	0.48
8:8:115:LYS:HB3	8:8:116:ASN:HB2	1.96	0.48
3:3:182:TRP:O	3:3:186:MET:N	2.45	0.48
5:5:124:TYR:H	5:5:156:LYS:HE2	1.78	0.48
5:5:260:TYR:HE2	5:5:321:GLY:HA2	1.78	0.48
6:6:86:LYS:HB2	7:7:450:GLU:OE2	2.13	0.48
8:8:221:ASP:OD2	8:8:338:THR:HA	2.14	0.48
9:9:207:CYS:O	9:9:368:TYR:N	2.44	0.48
4:4:273:MET:HB3	5:5:218:LEU:HD22	1.96	0.48
8:8:203:ASP:OD1	8:8:206:ARG:NH2	2.34	0.48
50:w:597:ASN:HB3	50:w:599:LYS:HZ3	1.78	0.48
2:2:620:ALA:O	2:2:625:LEU:N	2.47	0.48
5:5:209:HIS:O	5:5:212:ASN:ND2	2.47	0.48
5:5:250:VAL:HA	5:5:253:MET:HB2	1.96	0.48
6:6:30:GLU:OE2	6:6:54:TYR:OH	2.27	0.48
1:1:25:GLN:O	1:1:29:ASP:N	2.42	0.48
1:1:440:LEU:HD21	1:1:471:ILE:HG12	1.96	0.48
3:3:196:ILE:HG22	3:3:210:GLN:HB3	1.95	0.48
9:9:339:LEU:HD13	9:9:365:SER:HB3	1.95	0.48
49:u:9:PRO:HA	49:u:69:ARG:HE	1.78	0.48
2:2:439:ARG:O	2:2:443:CYS:N	2.43	0.48
2:2:476:GLU:OE1	2:2:513:LYS:NZ	2.47	0.48
7:7:328:ARG:NH1	7:7:330:GLN:HB2	2.29	0.48
50:w:232:ILE:HG22	50:w:233:GLU:HG3	1.95	0.48
1:1:16:ASN:HD22	1:1:19:LEU:HB2	1.78	0.48
1:1:365:PRO:HG2	1:1:370:LEU:HD22	1.95	0.48
3:3:29:LYS:HZ3	3:3:36:GLU:CD	2.22	0.48
3:3:172:LYS:HG2	3:3:188:ASP:OD2	2.14	0.48
6:6:149:THR:HA	7:7:503:THR:HG23	1.95	0.48
6:6:155:ARG:HD2	6:6:187:ILE:HG13	1.96	0.48
8:8:176:LYS:O	8:8:180:ALA:N	2.44	0.48
8:8:359:GLN:NE2	8:8:360:ASN:OD1	2.47	0.48
9:9:461:TYR:O	9:9:476:LEU:N	2.38	0.48
50:w:248:LYS:HB2	50:w:288:GLU:OE2	2.14	0.48
2:2:572:HIS:O	2:2:576:HIS:N	2.44	0.48
2:2:604:PRO:HD3	2:2:669:ARG:NH1	2.29	0.48
4:4:232:SER:HB3	5:5:220:LYS:NZ	2.29	0.48
9:9:262:ILE:HG21	9:9:289:PHE:HB3	1.94	0.48
1:1:405:GLU:HG3	1:1:406:ARG:HG3	1.95	0.47
1:1:414:VAL:HA	1:1:420:LYS:NZ	2.29	0.47
4:4:246:ARG:N	8:8:8:ASP:OD2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:130:THR:HB	5:5:133:LEU:HB2	1.97	0.47
8:8:19:ARG:HE	8:8:72:LEU:HD13	1.78	0.47
3:3:124:ARG:HE	3:3:155:ARG:HH22	1.61	0.47
4:4:110:ARG:NH1	8:8:104:GLN:HG3	2.28	0.47
4:4:237:VAL:HB	4:4:255:LEU:HD11	1.95	0.47
5:5:279:GLN:HA	5:5:282:GLN:HB3	1.96	0.47
7:7:253:PRO:O	7:7:257:ALA:N	2.46	0.47
50:w:277:GLN:HB2	50:w:301:GLN:HG3	1.95	0.47
50:w:514:ALA:HA	50:w:530:GLY:HA2	1.96	0.47
1:1:186:LEU:HD23	1:1:190:ARG:HH22	1.79	0.47
1:1:199:ASP:OD1	1:1:202:ARG:NH2	2.43	0.47
1:1:239:SER:HB2	2:2:731:GLU:OE2	2.15	0.47
1:1:404:CYS:HA	1:1:407:VAL:HG22	1.97	0.47
5:5:269:LYS:O	5:5:273:GLN:N	2.45	0.47
3:3:364:PRO:O	3:3:368:GLU:N	2.43	0.47
4:4:326:ARG:NH1	8:8:337:SER:HA	2.30	0.47
6:6:113:HIS:O	6:6:117:PHE:N	2.42	0.47
9:9:184:GLU:HG2	9:9:528:ARG:HG2	1.97	0.47
1:1:476:ARG:HE	2:2:791:TYR:HA	1.80	0.47
3:3:312:LEU:HD22	3:3:336:ALA:HB1	1.97	0.47
4:4:242:GLY:HA3	8:8:6:PHE:HD2	1.80	0.47
4:4:275:THR:HG23	4:4:279:PRO:HG3	1.95	0.47
4:4:365:GLN:O	7:7:537:ARG:NH1	2.47	0.47
6:6:21:TYR:HB2	7:7:259:GLU:OE2	2.15	0.47
7:7:515:SER:OG	7:7:516:ALA:N	2.45	0.47
8:8:309:GLU:OE2	8:8:331:LYS:NZ	2.43	0.47
1:1:174:TYR:O	1:1:227:SER:OG	2.30	0.47
1:1:210:ARG:HB3	1:1:212:HIS:HD2	1.79	0.47
1:1:535:GLU:OE2	4:4:304:SER:HB2	2.14	0.47
2:2:578:LEU:HA	2:2:622:ARG:NH1	2.29	0.47
6:6:114:PHE:HA	6:6:117:PHE:HB3	1.97	0.47
6:6:153:ILE:HG21	6:6:158:LEU:HB2	1.96	0.47
6:6:190:CYS:HB3	6:6:194:GLU:HG3	1.97	0.47
9:9:303:ASN:HD22	9:9:437:ASN:HB3	1.79	0.47
1:1:96:LEU:HG	1:1:148:PRO:HB2	1.97	0.47
1:1:549:GLN:O	1:1:553:ALA:N	2.45	0.47
5:5:125:TYR:H	5:5:156:LYS:NZ	2.13	0.47
6:6:155:ARG:NH2	6:6:167:ASP:OD1	2.47	0.47
1:1:429:PRO:O	1:1:433:SER:N	2.47	0.47
2:2:365:ASN:H	2:2:368:GLU:H	1.62	0.47
2:2:834:SER:HB2	2:2:843:VAL:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:51:LEU:HB3	6:6:88:MET:HB2	1.97	0.47
6:6:91:GLN:HA	6:6:94:GLN:HB2	1.97	0.47
8:8:19:ARG:HH22	8:8:47:GLU:HG2	1.78	0.47
1:1:372:ASN:HA	1:1:375:VAL:HB	1.97	0.47
2:2:760:LYS:O	2:2:765:VAL:N	2.49	0.47
6:6:153:ILE:HG12	6:6:157:LEU:HB3	1.97	0.47
9:9:261:ALA:O	9:9:265:THR:OG1	2.32	0.47
50:w:290:TYR:OH	50:w:354:THR:OG1	2.29	0.47
2:2:576:HIS:HA	2:2:580:SER:HB3	1.96	0.46
2:2:578:LEU:HG	2:2:622:ARG:HH12	1.80	0.46
2:2:789:ARG:HE	2:2:821:ILE:HG23	1.79	0.46
2:2:871:GLU:OE1	5:5:268:SER:OG	2.32	0.46
3:3:211:ARG:NH1	3:3:236:PHE:HB3	2.30	0.46
6:6:55:GLN:HE21	7:7:442:GLN:HG2	1.80	0.46
8:8:340:ARG:HB3	8:8:344:LYS:HB2	1.96	0.46
9:9:250:SER:HA	9:9:257:TYR:CZ	2.50	0.46
49:u:13:THR:HG21	49:u:29:VAL:HG11	1.97	0.46
2:2:395:PRO:O	2:2:399:GLN:N	2.45	0.46
5:5:218:LEU:O	5:5:222:SER:N	2.48	0.46
6:6:16:LYS:HZ2	7:7:295:GLU:HG2	1.80	0.46
8:8:144:LEU:HD21	8:8:184:VAL:HG22	1.96	0.46
9:9:411:SER:HA	9:9:414:ALA:HB3	1.97	0.46
1:1:540:ALA:HB2	4:4:303:LEU:HD22	1.97	0.46
4:4:338:ILE:HG13	4:4:339:VAL:H	1.80	0.46
7:7:421:LEU:O	7:7:443:GLN:NE2	2.49	0.46
1:1:82:ASN:HA	1:1:85:SER:HB3	1.97	0.46
2:2:666:GLU:HB2	2:2:667:ARG:HH11	1.80	0.46
2:2:817:THR:O	2:2:821:ILE:N	2.46	0.46
7:7:475:LEU:O	7:7:479:LEU:N	2.37	0.46
2:2:566:THR:HG23	2:2:594:LEU:HD22	1.97	0.46
4:4:106:PHE:N	8:8:97:GLU:OE1	2.48	0.46
4:4:259:TYR:H	5:5:228:HIS:CE1	2.33	0.46
7:7:461:ARG:HA	7:7:502:TRP:HE1	1.81	0.46
1:1:237:LEU:HD11	1:1:279:VAL:HG13	1.98	0.46
1:1:452:PHE:HA	1:1:455:LEU:HB3	1.98	0.46
2:2:714:PHE:HA	2:2:717:GLN:HB2	1.97	0.46
8:8:90:LEU:HD21	8:8:102:ARG:NH1	2.31	0.46
8:8:141:PRO:HA	8:8:144:LEU:HB2	1.98	0.46
9:9:370:TYR:HE1	9:9:384:ARG:HG3	1.81	0.46
50:w:433:VAL:HB	50:w:446:ASN:HB2	1.96	0.46
1:1:53:LYS:NZ	1:1:87:GLU:OE1	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:419:PHE:O	2:2:431:LEU:N	2.48	0.46
5:5:125:TYR:H	5:5:156:LYS:HZ1	1.62	0.46
1:1:201:LEU:HB2	1:1:228:MET:HE3	1.97	0.46
1:1:329:ILE:HG12	1:1:370:LEU:HD21	1.97	0.46
1:1:528:SER:OG	4:4:293:GLY:O	2.31	0.46
3:3:408:THR:HG23	3:3:409:LYS:HG2	1.97	0.46
5:5:345:GLN:HA	5:5:348:GLN:HB2	1.97	0.46
6:6:45:GLU:HB2	7:7:294:LEU:HD23	1.97	0.46
50:w:555:TYR:HD2	50:w:596:LYS:NZ	2.14	0.46
1:1:91:ARG:O	1:1:95:LYS:N	2.38	0.46
1:1:93:TYR:O	1:1:97:ALA:N	2.46	0.46
1:1:365:PRO:HB2	1:1:370:LEU:HB2	1.97	0.46
1:1:555:THR:OG1	4:4:228:ASN:ND2	2.41	0.46
4:4:329:MET:O	4:4:333:ASN:ND2	2.49	0.46
5:5:332:GLU:O	5:5:336:GLN:N	2.43	0.46
7:7:545:ARG:HA	7:7:548:HIS:HB3	1.98	0.46
8:8:57:ASP:OD2	8:8:58:LYS:HG3	2.16	0.46
8:8:172:LEU:HB3	8:8:174:ASP:OD2	2.16	0.46
9:9:336:GLN:HA	9:9:339:LEU:HD12	1.97	0.46
1:1:90:VAL:HG22	1:1:172:ARG:NH1	2.31	0.46
1:1:315:MET:SD	1:1:382:TYR:OH	2.62	0.46
1:1:323:LEU:HB2	1:1:387:VAL:HG11	1.97	0.46
1:1:572:ARG:NH1	4:4:128:ARG:NH1	2.47	0.46
2:2:354:LEU:HB3	2:2:374:ILE:HG23	1.97	0.46
2:2:868:GLU:OE1	4:4:367:GLN:NE2	2.48	0.46
4:4:227:GLN:O	5:5:216:TRP:NE1	2.49	0.46
5:5:148:VAL:HG12	5:5:168:ARG:HB3	1.98	0.46
7:7:388:LEU:HA	7:7:391:ARG:HB2	1.98	0.46
7:7:401:MET:HB2	7:7:408:VAL:HB	1.98	0.46
8:8:59:ASP:OD2	8:8:61:GLU:HG2	2.15	0.46
1:1:289:ALA:O	1:1:293:ALA:N	2.44	0.45
2:2:375:LYS:HB2	2:2:408:LEU:HD13	1.98	0.45
4:4:266:ARG:HH12	5:5:231:LEU:HD23	1.82	0.45
4:4:355:LEU:O	4:4:359:TYR:N	2.44	0.45
9:9:238:VAL:H	9:9:384:ARG:NH1	2.10	0.45
9:9:345:ARG:NH2	51:9:617:HOH:O	2.48	0.45
1:1:323:LEU:HD13	1:1:387:VAL:HG21	1.98	0.45
2:2:371:ILE:HA	2:2:374:ILE:HB	1.98	0.45
3:3:259:THR:HG21	3:3:328:CYS:HB3	1.97	0.45
3:3:283:GLN:O	3:3:287:THR:N	2.42	0.45
6:6:195:SER:HA	7:7:503:THR:HG22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:478:PHE:O	7:7:482:THR:N	2.42	0.45
7:7:529:HIS:HA	7:7:532:ASP:HB2	1.97	0.45
1:1:47:HIS:O	1:1:51:MET:N	2.39	0.45
1:1:53:LYS:CA	1:1:91:ARG:HH12	2.28	0.45
2:2:555:ILE:HG23	2:2:558:LYS:HE2	1.98	0.45
7:7:309:PRO:HA	7:7:312:GLN:HB3	1.98	0.45
9:9:314:GLY:O	9:9:322:ASN:ND2	2.44	0.45
1:1:181:ALA:CB	1:1:196:LYS:HZ1	2.29	0.45
2:2:410:ASP:OD1	2:2:485:ARG:NH2	2.49	0.45
2:2:576:HIS:ND1	2:2:584:GLN:OE1	2.40	0.45
4:4:170:MET:HA	4:4:173:ALA:HB3	1.97	0.45
6:6:15:LEU:O	6:6:20:ARG:NH1	2.50	0.45
5:5:141:GLN:HG2	5:5:147:SER:HB3	1.98	0.45
5:5:153:ASP:HB2	5:5:163:SER:HA	1.98	0.45
6:6:154:ASP:HB3	6:6:157:LEU:HB2	1.99	0.45
50:w:210:SER:HB2	50:w:221:ILE:HA	1.99	0.45
1:1:77:ILE:HG12	1:1:84:LYS:NZ	2.30	0.45
1:1:110:GLN:HE21	1:1:138:GLN:HB3	1.82	0.45
1:1:451:GLU:OE2	8:8:328:THR:OG1	2.32	0.45
2:2:874:PHE:HB2	5:5:272:GLN:HB3	1.99	0.45
6:6:8:ARG:O	6:6:12:GLY:N	2.46	0.45
7:7:408:VAL:O	7:7:412:LEU:N	2.48	0.45
8:8:292:ILE:HG12	8:8:332:VAL:HG22	1.99	0.45
1:1:95:LYS:HB3	1:1:151:LYS:HD3	1.99	0.45
1:1:448:GLN:HB2	8:8:324:LYS:HB3	1.97	0.45
2:2:417:ASN:OD1	2:2:441:ARG:NH1	2.50	0.45
2:2:487:GLN:HE22	2:2:506:ARG:HG2	1.81	0.45
2:2:681:LEU:O	2:2:685:VAL:N	2.43	0.45
3:3:38:LEU:HD21	3:3:252:HIS:NE2	2.32	0.45
3:3:51:VAL:O	3:3:54:ALA:N	2.49	0.45
5:5:245:LEU:HG	5:5:338:LEU:HD21	1.98	0.45
7:7:184:TRP:HZ3	7:7:243:GLN:HG2	1.82	0.45
8:8:250:ALA:HB2	8:8:279:LEU:HD21	1.97	0.45
9:9:391:MET:HB2	9:9:401:LEU:HD11	1.98	0.45
9:9:420:ARG:NH2	9:9:463:SER:OG	2.50	0.45
50:w:211:VAL:H	50:w:245:TRP:HZ2	1.65	0.45
50:w:291:LEU:HB3	50:w:310:TRP:HB2	1.98	0.45
1:1:129:LEU:O	1:1:134:GLY:N	2.36	0.45
1:1:472:VAL:HG22	1:1:484:ILE:HG21	1.98	0.45
1:1:551:GLN:O	4:4:228:ASN:ND2	2.49	0.45
3:3:248:THR:O	3:3:289:LYS:NZ	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:180:SER:O	6:6:188:PHE:N	2.43	0.45
8:8:356:ALA:O	8:8:360:ASN:ND2	2.49	0.45
1:1:88:ASP:O	1:1:92:ALA:N	2.50	0.45
4:4:144:VAL:HG11	4:4:216:ASN:HD21	1.82	0.45
8:8:52:CYS:HA	8:8:86:LEU:HB2	1.99	0.45
8:8:147:VAL:HG13	8:8:188:LEU:HD21	1.99	0.45
8:8:158:THR:O	8:8:162:HIS:N	2.39	0.45
50:w:468:ILE:HA	50:w:485:GLY:H	1.82	0.45
1:1:43:TRP:HZ2	1:1:80:GLN:HB2	1.82	0.45
1:1:566:GLN:HG3	1:1:569:LEU:HD23	1.98	0.45
2:2:399:GLN:HA	2:2:402:LEU:HB3	1.98	0.45
2:2:426:GLU:HG2	2:2:430:ASN:HD21	1.82	0.45
2:2:455:PHE:HA	2:2:458:ILE:HB	1.98	0.45
4:4:311:GLU:HB2	4:4:317:LYS:HB3	1.98	0.45
6:6:15:LEU:HD22	6:6:45:GLU:HG2	1.97	0.45
6:6:82:PHE:HB3	6:6:110:GLU:OE2	2.17	0.45
7:7:275:VAL:HG12	7:7:279:ARG:HH11	1.82	0.45
8:8:17:GLU:HA	8:8:38:LEU:HD21	1.99	0.45
8:8:162:HIS:HA	8:8:165:LEU:HB2	1.98	0.45
9:9:282:LYS:NZ	9:9:513:ASP:OD1	2.47	0.45
1:1:551:GLN:O	1:1:555:THR:OG1	2.29	0.44
1:1:567:ARG:O	1:1:571:ARG:N	2.42	0.44
3:3:169:LEU:O	3:3:173:LEU:N	2.44	0.44
5:5:269:LYS:HE2	5:5:273:GLN:HE21	1.83	0.44
6:6:90:ASP:O	6:6:94:GLN:N	2.50	0.44
9:9:195:LEU:HD22	9:9:502:ARG:HB2	1.99	0.44
1:1:125:GLU:O	1:1:129:LEU:N	2.49	0.44
2:2:556:TYR:CD1	2:2:559:ASP:HB3	2.53	0.44
3:3:32:TYR:HB3	3:3:59:LYS:HD2	1.99	0.44
3:3:111:ARG:O	3:3:115:ASP:N	2.51	0.44
5:5:336:GLN:HB3	5:5:340:LYS:HZ1	1.81	0.44
7:7:271:TYR:H	7:7:279:ARG:HH22	1.66	0.44
8:8:48:ALA:HB1	8:8:73:ILE:HG22	2.00	0.44
8:8:55:GLU:OE2	8:8:92:LYS:NZ	2.26	0.44
8:8:70:LEU:HD21	8:8:102:ARG:HB3	1.98	0.44
8:8:155:ASN:O	8:8:159:GLU:N	2.36	0.44
50:w:348:THR:HG23	50:w:364:SER:HB3	1.99	0.44
2:2:799:TYR:HD1	2:2:799:TYR:HA	1.72	0.44
3:3:131:LEU:O	3:3:135:ALA:N	2.47	0.44
5:5:39:VAL:HG13	5:5:203:ILE:HG23	1.99	0.44
5:5:70:LEU:HD23	5:5:112:ILE:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:8:168:LEU:HA	8:8:171:ALA:HB3	1.99	0.44
9:9:464:ARG:NH1	51:9:639:HOH:O	2.50	0.44
9:9:464:ARG:HH11	9:9:467:VAL:C	2.25	0.44
9:9:498:TRP:NE1	51:9:723:HOH:O	2.49	0.44
1:1:277:ASN:HD21	1:1:359:LEU:HD22	1.82	0.44
2:2:373:LYS:HB2	2:2:419:PHE:CE2	2.52	0.44
3:3:124:ARG:CG	3:3:155:ARG:HH12	2.28	0.44
3:3:221:VAL:HG13	3:3:225:HIS:HB2	1.99	0.44
6:6:91:GLN:H	7:7:445:LYS:HD3	1.82	0.44
6:6:191:SER:H	6:6:194:GLU:HG3	1.82	0.44
8:8:143:GLU:O	8:8:147:VAL:N	2.49	0.44
9:9:282:LYS:O	9:9:514:GLY:N	2.44	0.44
50:w:272:GLN:NE2	50:w:312:ILE:O	2.39	0.44
50:w:333:LYS:HD2	50:w:375:TRP:HD1	1.82	0.44
2:2:487:GLN:NE2	2:2:502:VAL:O	2.50	0.44
3:3:93:LYS:HB3	3:3:96:GLU:OE2	2.18	0.44
3:3:100:THR:HG22	3:3:104:MET:HE3	1.98	0.44
3:3:108:ARG:HH12	3:3:112:MET:HA	1.83	0.44
6:6:65:VAL:HA	6:6:68:GLN:HB2	1.99	0.44
7:7:275:VAL:HG12	7:7:279:ARG:NH1	2.32	0.44
7:7:507:SER:HB3	7:7:512:GLU:HB3	2.00	0.44
9:9:190:LEU:HB3	9:9:500:ILE:HG12	2.00	0.44
2:2:521:ARG:NH1	2:2:542:GLU:HB3	2.33	0.44
4:4:179:LEU:HD21	5:5:102:GLU:HB3	2.00	0.44
4:4:217:PRO:HG3	4:4:241:MET:HE3	1.99	0.44
4:4:300:GLN:HE22	4:4:331:LEU:HD22	1.81	0.44
6:6:136:ASP:O	6:6:140:LYS:N	2.45	0.44
8:8:234:GLY:O	8:8:240:LEU:N	2.50	0.44
1:1:403:LEU:HB3	1:1:439:LEU:HD13	1.99	0.44
4:4:153:ASN:N	4:4:187:GLU:OE2	2.51	0.44
50:w:292:VAL:HG22	50:w:309:ILE:HG23	1.99	0.44
1:1:431:LEU:O	1:1:435:THR:N	2.51	0.44
7:7:470:MET:HB2	7:7:513:PHE:HD2	1.81	0.44
8:8:165:LEU:HB3	8:8:185:MET:HB2	2.00	0.44
8:8:204:ALA:HB2	8:8:232:LEU:HD22	2.00	0.44
50:w:417:ASP:OD2	50:w:432:LYS:NZ	2.31	0.44
2:2:583:TYR:HA	2:2:586:ARG:HE	1.83	0.44
49:u:26:ILE:HG22	49:u:49:PHE:HA	1.99	0.44
50:w:251:TYR:HD1	50:w:264:GLY:HA3	1.83	0.44
1:1:91:ARG:HA	1:1:94:LEU:HB2	1.99	0.43
1:1:210:ARG:HB3	1:1:212:HIS:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:384:VAL:HA	1:1:385:PRO:HD3	1.86	0.43
1:1:500:ALA:HA	1:1:520:ARG:NH1	2.24	0.43
2:2:867:VAL:HB	5:5:265:ARG:HD2	1.99	0.43
3:3:19:VAL:HG11	3:3:45:LEU:HA	1.99	0.43
5:5:300:ASP:HA	5:5:303:LYS:HB2	1.99	0.43
6:6:14:LEU:HD11	6:6:25:ASN:HB3	1.99	0.43
6:6:33:VAL:HG11	6:6:69:ILE:HG13	2.01	0.43
6:6:125:MET:HB3	6:6:128:LEU:HG	2.00	0.43
7:7:190:PHE:HB3	7:7:194:PHE:CE2	2.53	0.43
8:8:363:LYS:HA	8:8:366:ASN:HB2	2.00	0.43
50:w:329:TRP:CD2	50:w:330:PRO:HA	2.53	0.43
1:1:13:LYS:NZ	1:1:39:LYS:HZ2	2.13	0.43
1:1:230:LEU:HA	1:1:233:ARG:HG2	2.00	0.43
2:2:449:GLU:O	2:2:453:GLU:N	2.46	0.43
4:4:128:ARG:HE	5:5:79:THR:HB	1.83	0.43
6:6:213:ILE:O	7:7:534:LYS:NZ	2.48	0.43
9:9:266:ILE:HG23	9:9:504:ILE:HD12	2.01	0.43
1:1:45:LYS:N	1:1:48:GLU:OE1	2.38	0.43
2:2:850:THR:OG1	4:4:353:ASP:OD2	2.35	0.43
4:4:137:ILE:HB	4:4:159:HIS:HB2	1.99	0.43
4:4:310:ALA:HB1	4:4:316:GLY:HA3	2.00	0.43
6:6:102:ILE:HG12	6:6:105:LEU:HD12	1.99	0.43
6:6:159:ALA:HB2	6:6:170:LEU:HD13	2.01	0.43
9:9:204:VAL:N	9:9:370:TYR:O	2.51	0.43
9:9:532:ILE:HD12	9:9:536:THR:HB	2.00	0.43
1:1:508:GLY:HA2	1:1:509:PRO:HD3	1.85	0.43
2:2:460:GLN:HA	2:2:672:PRO:HA	2.00	0.43
3:3:138:GLN:HE21	3:3:148:ALA:HB2	1.82	0.43
3:3:248:THR:HG21	3:3:282:GLN:HA	2.00	0.43
5:5:303:LYS:HA	5:5:306:LYS:NZ	2.33	0.43
1:1:69:GLU:HA	1:1:72:TYR:HD2	1.82	0.43
1:1:274:ASN:HD21	1:1:299:LEU:HA	1.84	0.43
1:1:495:SER:HA	1:1:496:ASP:HA	1.77	0.43
2:2:573:ILE:HG23	2:2:585:ALA:HB1	2.01	0.43
5:5:276:GLN:O	5:5:280:ARG:N	2.44	0.43
7:7:228:LEU:HD22	7:7:232:HIS:HE2	1.84	0.43
8:8:342:PHE:HA	8:8:345:GLN:HB3	2.00	0.43
9:9:517:LEU:HD23	9:9:519:MET:HB2	2.01	0.43
1:1:206:SER:HA	1:1:209:GLN:HB2	2.00	0.43
3:3:265:LYS:HD3	3:3:269:LYS:HE2	2.00	0.43
3:3:278:VAL:HA	3:3:283:GLN:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:164:ASP:OD2	4:4:205:LEU:HD11	2.17	0.43
6:6:40:ASN:HA	6:6:72:LYS:HZ2	1.83	0.43
7:7:263:HIS:HA	7:7:266:TYR:HB3	2.00	0.43
7:7:284:LEU:HD13	7:7:299:LEU:HD13	2.01	0.43
8:8:159:GLU:O	8:8:163:THR:N	2.42	0.43
9:9:491:ASN:ND2	51:9:691:HOH:O	2.42	0.43
9:9:521:ASP:OD2	9:9:524:LYS:HB2	2.18	0.43
49:u:12:VAL:HG13	49:u:13:THR:H	1.83	0.43
1:1:541:HIS:HA	1:1:544:GLN:HB3	2.01	0.43
2:2:373:LYS:HA	2:2:376:PHE:HB3	2.01	0.43
2:2:503:TYR:OH	2:2:572:HIS:NE2	2.37	0.43
3:3:316:GLU:OE2	3:3:336:ALA:HB3	2.18	0.43
8:8:276:LYS:HZ3	8:8:302:GLN:HB2	1.84	0.43
3:3:330:GLU:HA	3:3:333:ILE:HB	2.00	0.43
5:5:122:SER:N	5:5:123:THR:OG1	2.37	0.43
8:8:322:TYR:N	8:8:334:VAL:O	2.50	0.43
50:w:410:ARG:HE	50:w:412:LEU:HD21	1.83	0.43
2:2:351:ILE:HG22	2:2:355:GLN:HE22	1.84	0.43
2:2:564:ILE:O	2:2:568:ALA:N	2.49	0.43
3:3:26:LEU:H	3:3:68:HIS:CE1	2.37	0.43
5:5:216:TRP:CE2	5:5:220:LYS:NZ	2.87	0.43
8:8:282:PHE:CG	8:8:338:THR:HB	2.53	0.43
50:w:474:GLU:OE2	50:w:523:GLY:HA2	2.19	0.43
1:1:198:CYS:HB3	1:1:202:ARG:NH1	2.33	0.43
1:1:440:LEU:HD11	1:1:471:ILE:HA	2.00	0.43
2:2:658:ARG:HA	2:2:659:ASN:HA	1.71	0.43
4:4:116:PRO:HB3	5:5:214:LEU:HD22	2.00	0.43
4:4:129:ARG:HD3	4:4:133:ALA:HA	2.01	0.43
6:6:151:GLN:N	7:7:504:SER:O	2.52	0.43
7:7:363:GLN:HA	7:7:419:LYS:HD3	2.01	0.43
9:9:195:LEU:HD23	9:9:498:TRP:HB3	2.00	0.43
50:w:484:HIS:N	50:w:491:SER:O	2.51	0.43
1:1:7:ARG:NH2	1:1:48:GLU:OE2	2.48	0.42
3:3:208:LEU:HA	3:3:211:ARG:HD2	2.02	0.42
3:3:261:VAL:HG21	3:3:273:VAL:HG21	2.00	0.42
4:4:269:VAL:O	4:4:273:MET:N	2.41	0.42
5:5:260:TYR:CE2	5:5:321:GLY:HA2	2.53	0.42
7:7:386:ILE:HG23	7:7:390:LEU:HB2	2.01	0.42
8:8:56:ASP:OD2	8:8:102:ARG:NH2	2.52	0.42
8:8:91:VAL:HG21	8:8:129:LYS:HE3	2.01	0.42
8:8:156:LEU:HA	8:8:159:GLU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:9:526:MET:SD	9:9:528:ARG:NH2	2.92	0.42
50:w:555:TYR:H	50:w:596:LYS:NZ	2.16	0.42
1:1:173:GLN:O	1:1:158:ARG:NH2	2.52	0.42
3:3:156:VAL:HG21	3:3:191:ARG:HH12	1.82	0.42
6:6:20:ARG:CZ	7:7:292:LYS:HZ1	2.32	0.42
8:8:219:LEU:HD21	8:8:275:ALA:HB1	2.01	0.42
8:8:239:ASP:OD2	8:8:260:LYS:NZ	2.39	0.42
2:2:392:TYR:HD1	2:2:457:LYS:HB3	1.84	0.42
6:6:161:MET:HE2	7:7:494:LYS:HG3	2.01	0.42
8:8:351:TYR:O	8:8:355:ASN:N	2.36	0.42
9:9:369:ARG:HD3	9:9:371:ARG:NH1	2.31	0.42
1:1:229:HIS:O	1:1:232:THR:OG1	2.33	0.42
1:1:342:LEU:HD23	2:2:706:ARG:NH1	2.34	0.42
1:1:419:GLU:OE2	1:1:420:LYS:HG3	2.19	0.42
2:2:466:SER:HB2	2:2:468:GLU:HG3	2.01	0.42
2:2:646:LEU:HD11	2:2:677:ILE:HG13	2.02	0.42
4:4:123:VAL:HG21	5:5:213:VAL:HB	2.02	0.42
4:4:175:ASN:HB3	5:5:102:GLU:OE2	2.19	0.42
4:4:304:SER:OG	8:8:348:GLN:NE2	2.37	0.42
1:1:193:GLU:OE2	1:1:196:LYS:NZ	2.53	0.42
2:2:580:SER:OG	2:2:581:ARG:N	2.53	0.42
4:4:135:ARG:HH21	4:4:194:ALA:HB1	1.83	0.42
4:4:263:ASP:HA	4:4:266:ARG:HE	1.85	0.42
6:6:113:HIS:HA	7:7:495:HIS:CE1	2.54	0.42
7:7:317:TYR:OH	7:7:363:GLN:OE1	2.36	0.42
8:8:66:SER:HA	8:8:69:SER:HB3	2.01	0.42
1:1:139:ASP:HA	1:1:142:ASP:HB3	2.02	0.42
2:2:322:THR:HG22	2:2:324:ILE:HG12	2.02	0.42
3:3:81:LEU:HD12	3:3:84:LEU:HD21	2.01	0.42
5:5:170:THR:HG22	5:5:173:LEU:H	1.84	0.42
8:8:19:ARG:NH1	8:8:47:GLU:O	2.42	0.42
1:1:401:LEU:HD22	1:1:458:LEU:HB3	2.01	0.42
2:2:772:ALA:HA	2:2:775:VAL:HB	2.01	0.42
6:6:40:ASN:HA	6:6:72:LYS:NZ	2.35	0.42
6:6:146:VAL:HG12	6:6:189:ILE:HG21	2.02	0.42
8:8:108:ASN:HB2	8:8:114:ASP:HB2	2.01	0.42
8:8:189:LEU:HD21	8:8:232:LEU:HD21	2.02	0.42
9:9:317:LEU:HD12	9:9:470:SER:HB3	2.01	0.42
50:w:326:SER:HA	50:w:327:ALA:HA	1.59	0.42
1:1:482:VAL:O	2:2:795:TYR:OH	2.38	0.42
4:4:347:LEU:O	4:4:351:ILE:N	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:6:95:GLU:HA	6:6:100:ARG:HB2	2.02	0.42
1:1:196:LYS:HE3	1:1:196:LYS:HB3	1.82	0.42
1:1:256:ILE:O	1:1:260:PHE:N	2.39	0.42
2:2:430:ASN:HB3	2:2:433:ASN:H	1.85	0.42
2:2:503:TYR:HH	2:2:572:HIS:HE2	1.62	0.42
6:6:36:GLN:HB3	6:6:72:LYS:HE2	2.01	0.42
6:6:64:THR:O	6:6:68:GLN:N	2.46	0.42
8:8:273:ASN:HA	8:8:276:LYS:HB3	2.01	0.42
9:9:179:TRP:HZ2	9:9:536:THR:HG21	1.84	0.42
9:9:190:LEU:O	9:9:496:ASN:ND2	2.36	0.42
50:w:569:VAL:O	50:w:587:TRP:N	2.45	0.42
2:2:549:GLU:OE2	2:2:550:ARG:HG3	2.19	0.42
2:2:644:GLU:OE2	2:2:653:ARG:NH2	2.53	0.42
2:2:698:MET:HA	2:2:701:HIS:HD2	1.85	0.42
6:6:52:LYS:NZ	6:6:56:PHE:HB2	2.35	0.42
8:8:246:SER:OG	8:8:254:LYS:O	2.37	0.42
1:1:558:LEU:HD22	5:5:216:TRP:CD1	2.55	0.41
2:2:660:GLN:O	2:2:664:LYS:N	2.52	0.41
2:2:714:PHE:O	2:2:718:LEU:N	2.51	0.41
3:3:176:GLU:OE1	3:3:181:ASN:ND2	2.48	0.41
3:3:218:SER:HA	3:3:225:HIS:CE1	2.54	0.41
3:3:420:MET:HG2	7:7:543:PHE:CD2	2.54	0.41
4:4:264:THR:O	4:4:268:GLY:N	2.48	0.41
5:5:256:ASP:O	5:5:328:GLN:NE2	2.53	0.41
8:8:159:GLU:HA	8:8:162:HIS:HB2	2.01	0.41
9:9:222:VAL:HG23	9:9:223:LYS:HG3	2.01	0.41
50:w:292:VAL:HG21	50:w:334:TRP:HE1	1.85	0.41
1:1:7:ARG:HA	1:1:51:MET:HE1	2.01	0.41
1:1:165:ARG:NE	1:1:167:ASN:OD1	2.44	0.41
1:1:402:LYS:HD3	1:1:406:ARG:HH22	1.85	0.41
1:1:432:GLN:HE22	1:1:462:VAL:HG23	1.85	0.41
3:3:50:MET:HG3	3:3:178:LEU:HB3	2.01	0.41
4:4:153:ASN:HB2	5:5:51:LYS:HE3	2.02	0.41
4:4:304:SER:OG	8:8:352:ASP:OD2	2.35	0.41
5:5:297:PRO:HB2	5:5:299:GLU:HG3	2.02	0.41
8:8:144:LEU:HA	8:8:147:VAL:HB	2.00	0.41
50:w:290:TYR:HH	50:w:354:THR:HG1	1.59	0.41
50:w:384:PHE:HE1	50:w:399:MET:HB2	1.85	0.41
4:4:130:ASN:ND2	5:5:109:HIS:O	2.53	0.41
4:4:326:ARG:HH12	8:8:337:SER:HA	1.86	0.41
6:6:138:VAL:O	6:6:142:ILE:N	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:7:327:ARG:HA	7:7:329:TYR:CZ	2.55	0.41
1:1:335:ARG:HD2	1:1:341:LEU:HD21	2.01	0.41
1:1:438:ARG:HE	1:1:510:HIS:CD2	2.38	0.41
2:2:378:ILE:O	2:2:382:LEU:N	2.40	0.41
2:2:670:GLN:HA	2:2:671:VAL:HA	1.91	0.41
2:2:867:VAL:O	2:2:871:GLU:N	2.52	0.41
5:5:38:GLN:O	5:5:76:LEU:N	2.40	0.41
1:1:278:LYS:HA	1:1:299:LEU:HD12	2.03	0.41
1:1:328:SER:HB2	1:1:427:TYR:CD2	2.55	0.41
1:1:387:VAL:HA	1:1:390:LEU:HB3	2.02	0.41
1:1:391:TYR:O	1:1:395:GLU:N	2.48	0.41
1:1:587:ILE:HG22	1:1:591:LYS:HZ2	1.86	0.41
2:2:390:ALA:HA	2:2:391:THR:HA	1.90	0.41
7:7:199:GLN:NE2	7:7:260:TYR:OH	2.37	0.41
49:u:22:ARG:HH21	49:u:26:ILE:HG12	1.85	0.41
1:1:135:GLU:O	1:1:137:THR:N	2.50	0.41
1:1:532:LYS:NZ	4:4:331:LEU:HD11	2.35	0.41
1:1:551:GLN:HE21	4:4:228:ASN:HB3	1.85	0.41
5:5:230:LEU:O	5:5:234:ALA:N	2.49	0.41
9:9:212:TYR:HB2	9:9:340:LYS:HD2	2.02	0.41
50:w:223:TRP:NE1	50:w:225:ASP:OD1	2.50	0.41
50:w:289:ARG:NH2	50:w:337:ASP:O	2.54	0.41
50:w:535:ASN:HA	50:w:536:GLY:HA2	1.83	0.41
1:1:445:GLN:HB3	1:1:515:PRO:HA	2.02	0.41
1:1:537:ILE:HA	1:1:543:LEU:HD22	2.01	0.41
2:2:610:ASN:HB3	2:2:645:LEU:HD13	2.03	0.41
3:3:6:LEU:HD21	3:3:204:PRO:HB3	2.03	0.41
3:3:108:ARG:HB2	3:3:137:PHE:CZ	2.56	0.41
3:3:117:LEU:HD13	3:3:126:GLU:OE2	2.20	0.41
3:3:135:ALA:O	3:3:164:ASN:ND2	2.49	0.41
5:5:315:ASP:HA	5:5:318:LEU:HB3	2.03	0.41
7:7:215:LEU:HD11	7:7:225:HIS:CE1	2.56	0.41
1:1:77:ILE:HB	1:1:158:ARG:HH22	1.86	0.41
1:1:296:LEU:HB3	1:1:329:ILE:HG13	2.02	0.41
1:1:300:TYR:CZ	1:1:307:ARG:NH1	2.87	0.41
2:2:463:ASP:O	2:2:466:SER:OG	2.30	0.41
3:3:223:PHE:O	3:3:225:HIS:N	2.48	0.41
5:5:196:HIS:HB2	5:5:323:ILE:HG13	2.03	0.41
7:7:488:ILE:HG22	7:7:491:LEU:HB2	2.03	0.41
8:8:121:TYR:HA	8:8:124:TYR:HB3	2.02	0.41
1:1:412:ASN:OD1	1:1:415:ARG:NH1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:404:CYS:HA	2:2:407:GLU:HB3	2.03	0.41
2:2:430:ASN:OD1	2:2:432:GLN:NE2	2.52	0.41
2:2:574:TYR:HA	2:2:615:GLN:NE2	2.35	0.41
3:3:35:LYS:HA	3:3:38:LEU:HD23	2.03	0.41
3:3:175:SER:HA	3:3:178:LEU:HB2	2.03	0.41
4:4:144:VAL:HG12	4:4:149:VAL:HG22	2.03	0.41
5:5:40:GLN:HB2	5:5:75:ARG:HD3	2.01	0.41
6:6:44:LEU:HD23	7:7:294:LEU:HD13	2.02	0.41
6:6:72:LYS:HD2	6:6:72:LYS:HA	1.88	0.41
8:8:61:GLU:OE2	8:8:98:ARG:NH1	2.54	0.41
8:8:207:CYS:HA	8:8:210:ARG:HB2	2.02	0.41
8:8:223:LEU:HA	8:8:228:PRO:HG2	2.03	0.41
9:9:224:ASN:ND2	51:9:732:HOH:O	2.54	0.41
1:1:243:MET:HA	2:2:726:LEU:HB2	2.03	0.41
2:2:716:HIS:HA	2:2:719:ARG:HD3	2.03	0.41
4:4:304:SER:HA	4:4:307:LEU:HB2	2.03	0.41
7:7:270:GLY:HA2	7:7:279:ARG:HH22	1.86	0.41
7:7:274:LEU:HD11	7:7:308:VAL:HG11	2.02	0.41
8:8:219:LEU:HD13	8:8:247:ALA:HA	2.03	0.41
9:9:458:LYS:HG2	9:9:480:GLN:HA	2.01	0.41
50:w:213:PHE:HD2	50:w:603:CYS:HB2	1.86	0.41
50:w:586:LEU:HD23	50:w:594:LEU:HD22	2.02	0.41
1:1:236:GLN:NE2	1:1:245:LEU:O	2.54	0.40
1:1:250:PHE:HD1	1:1:358:LEU:HD22	1.85	0.40
1:1:474:ALA:HB1	1:1:479:ASP:HB2	2.02	0.40
1:1:579:LYS:HB3	5:5:115:LEU:HD11	2.03	0.40
2:2:375:LYS:HZ3	2:2:407:GLU:CD	2.28	0.40
2:2:434:VAL:HA	2:2:435:ASP:HA	1.83	0.40
2:2:503:TYR:CE1	2:2:549:GLU:HA	2.56	0.40
2:2:605:VAL:O	2:2:609:TYR:N	2.46	0.40
3:3:21:PRO:HG2	3:3:47:ASP:HA	2.02	0.40
3:3:123:PHE:HB2	3:3:126:GLU:HB3	2.03	0.40
4:4:196:GLY:N	4:4:222:VAL:O	2.54	0.40
7:7:487:ARG:HA	7:7:488:ILE:HA	1.76	0.40
9:9:371:ARG:HB2	9:9:373:TRP:CH2	2.56	0.40
50:w:382:ILE:O	50:w:399:MET:N	2.54	0.40
1:1:350:GLU:O	1:1:354:ARG:N	2.49	0.40
1:1:412:ASN:HA	1:1:415:ARG:HD2	2.02	0.40
2:2:776:ARG:O	2:2:780:VAL:N	2.54	0.40
5:5:68:LEU:HA	5:5:116:HIS:HA	2.03	0.40
5:5:76:LEU:HD13	5:5:117:VAL:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:8:61:GLU:HG2	8:8:98:ARG:HH12	1.87	0.40
49:u:12:VAL:CG1	49:u:33:ARG:HH11	2.33	0.40
50:w:451:ARG:HH22	50:w:501:GLY:HA2	1.84	0.40
1:1:13:LYS:HZ3	1:1:35:MET:CE	2.34	0.40
1:1:47:HIS:HA	1:1:50:ILE:HB	2.03	0.40
1:1:65:HIS:CE1	1:1:68:LYS:HG3	2.56	0.40
4:4:163:GLU:HA	4:4:164:ASP:HA	1.71	0.40
4:4:232:SER:H	5:5:220:LYS:HE2	1.87	0.40
5:5:122:SER:HB2	5:5:123:THR:HA	2.04	0.40
9:9:262:ILE:HA	9:9:297:PHE:HZ	1.85	0.40
49:u:11:ASP:OD2	49:u:66:LEU:HG	2.20	0.40
50:w:376:SER:HB3	50:w:381:ILE:HB	2.04	0.40
50:w:385:TRP:CD2	50:w:418:CYS:HB3	2.56	0.40
1:1:164:LEU:HA	1:1:213:ASN:HB2	2.04	0.40
1:1:445:GLN:HG3	1:1:515:PRO:HG3	2.03	0.40
2:2:821:ILE:O	2:2:825:MET:N	2.50	0.40
3:3:309:GLN:HB3	3:3:360:LEU:HD21	2.04	0.40
4:4:106:PHE:HB3	4:4:147:HIS:HE1	1.87	0.40
4:4:199:ILE:HG12	4:4:252:PHE:CD2	2.56	0.40
7:7:493:PHE:O	7:7:497:MET:N	2.50	0.40
8:8:128:ILE:HG12	8:8:168:LEU:HD13	2.03	0.40
8:8:255:PHE:O	8:8:259:ASN:N	2.54	0.40
50:w:363:LYS:HD2	50:w:404:ARG:HH21	1.87	0.40
5:5:125:TYR:CD2	5:5:128:PHE:HB2	2.57	0.40
9:9:182:ILE:HG21	9:9:511:GLN:HG3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	1	598/1362 (44%)	530 (89%)	67 (11%)	1 (0%)	43 77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	2	556/843 (66%)	507 (91%)	48 (9%)	1 (0%)	43	77
3	3	418/445 (94%)	348 (83%)	64 (15%)	6 (1%)	9	40
4	4	270/364 (74%)	230 (85%)	40 (15%)	0	100	100
5	5	322/352 (92%)	272 (84%)	50 (16%)	0	100	100
6	6	214/218 (98%)	193 (90%)	21 (10%)	0	100	100
7	7	371/564 (66%)	329 (89%)	41 (11%)	1 (0%)	36	72
8	8	364/374 (97%)	301 (83%)	63 (17%)	0	100	100
9	9	350/368 (95%)	325 (93%)	23 (7%)	2 (1%)	21	59
12	G	156/158 (99%)	139 (89%)	17 (11%)	0	100	100
13	H	139/141 (99%)	126 (91%)	11 (8%)	2 (1%)	9	40
14	I	261/263 (99%)	227 (87%)	31 (12%)	3 (1%)	11	46
15	J	51/53 (96%)	46 (90%)	5 (10%)	0	100	100
16	K	180/182 (99%)	165 (92%)	14 (8%)	1 (1%)	21	59
17	L	135/137 (98%)	114 (84%)	21 (16%)	0	100	100
19	P	264/266 (99%)	212 (80%)	48 (18%)	4 (2%)	8	39
20	Q	140/142 (99%)	124 (89%)	16 (11%)	0	100	100
21	R	139/141 (99%)	125 (90%)	14 (10%)	0	100	100
22	S	420/422 (100%)	366 (87%)	54 (13%)	0	100	100
23	U	189/191 (99%)	173 (92%)	15 (8%)	1 (0%)	24	63
24	V	57/59 (97%)	49 (86%)	8 (14%)	0	100	100
25	W	73/75 (97%)	65 (89%)	8 (11%)	0	100	100
26	X	188/190 (99%)	166 (88%)	17 (9%)	5 (3%)	4	25
27	Y	82/84 (98%)	74 (90%)	8 (10%)	0	100	100
28	Z	148/150 (99%)	143 (97%)	5 (3%)	0	100	100
29	a	127/129 (98%)	120 (94%)	7 (6%)	0	100	100
30	b	80/82 (98%)	69 (86%)	9 (11%)	2 (2%)	4	26
31	c	224/226 (99%)	205 (92%)	19 (8%)	0	100	100
32	d	15/17 (88%)	15 (100%)	0	0	100	100
33	e	124/126 (98%)	111 (90%)	12 (10%)	1 (1%)	16	54
34	f	206/208 (99%)	177 (86%)	27 (13%)	2 (1%)	12	48
35	g	225/227 (99%)	203 (90%)	20 (9%)	2 (1%)	14	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	h	102/104 (98%)	94 (92%)	8 (8%)	0	100	100
37	i	213/215 (99%)	188 (88%)	25 (12%)	0	100	100
38	j	134/136 (98%)	117 (87%)	16 (12%)	1 (1%)	18	56
39	k	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
40	l	62/64 (97%)	58 (94%)	4 (6%)	0	100	100
41	m	311/313 (99%)	271 (87%)	40 (13%)	0	100	100
42	n	125/127 (98%)	106 (85%)	17 (14%)	2 (2%)	7	37
43	o	204/206 (99%)	173 (85%)	29 (14%)	2 (1%)	12	48
44	p	69/71 (97%)	48 (70%)	21 (30%)	0	100	100
45	q	235/237 (99%)	211 (90%)	22 (9%)	2 (1%)	14	50
46	r	122/124 (98%)	97 (80%)	23 (19%)	2 (2%)	7	37
47	s	129/131 (98%)	110 (85%)	18 (14%)	1 (1%)	16	54
48	t	96/98 (98%)	76 (79%)	19 (20%)	1 (1%)	12	48
49	u	74/636 (12%)	61 (82%)	12 (16%)	1 (1%)	9	40
50	w	401/1121 (36%)	335 (84%)	66 (16%)	0	100	100
All	All	9460/12241 (77%)	8286 (88%)	1128 (12%)	46 (0%)	26	63

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	3	51	VAL
13	H	42	ILE
14	I	12	VAL
26	X	17	ASP
30	b	42	VAL
34	f	203	PHE
42	n	15	PHE
45	q	69	THR
45	q	152	ASP
48	t	44	HIS
1	1	166	ASN
3	3	50	MET
3	3	92	VAL
9	9	377	ASN
26	X	18	GLU
34	f	202	TYR
43	o	10	LYS

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Mol	Chain	Res	Type
46	r	118	SER
3	3	238	TYR
7	7	423	PRO
13	H	41	MET
14	I	11	ARG
23	U	80	GLY
30	b	41	LYS
49	u	9	PRO
9	9	427	ARG
19	P	40	ASN
19	P	166	LEU
38	j	128	ARG
42	n	14	LYS
43	o	9	HIS
46	r	119	GLN
2	2	387	PRO
19	P	47	LEU
19	P	164	ASP
26	X	190	PRO
26	X	76	GLN
26	X	107	LYS
35	g	202	LYS
47	s	30	PRO
3	3	246	ILE
14	I	150	PRO
16	K	148	ILE
33	e	95	ILE
35	g	213	PRO
3	3	28	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	1	551/1245 (44%)	547 (99%)	4 (1%)	76 81
2	2	503/750 (67%)	501 (100%)	2 (0%)	84 84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	3	384/406 (95%)	377 (98%)	7 (2%)	51	68
4	4	239/282 (85%)	238 (100%)	1 (0%)	84	84
5	5	293/311 (94%)	292 (100%)	1 (0%)	86	85
6	6	190/193 (98%)	190 (100%)	0	100	100
7	7	342/516 (66%)	340 (99%)	2 (1%)	78	83
8	8	327/335 (98%)	325 (99%)	2 (1%)	78	83
9	9	320/331 (97%)	319 (100%)	1 (0%)	86	85
12	G	142/142 (100%)	141 (99%)	1 (1%)	76	81
13	H	117/117 (100%)	117 (100%)	0	100	100
14	I	225/225 (100%)	225 (100%)	0	100	100
15	J	47/47 (100%)	47 (100%)	0	100	100
16	K	157/157 (100%)	157 (100%)	0	100	100
17	L	119/119 (100%)	117 (98%)	2 (2%)	53	69
19	P	238/238 (100%)	235 (99%)	3 (1%)	61	74
20	Q	114/114 (100%)	114 (100%)	0	100	100
21	R	113/113 (100%)	112 (99%)	1 (1%)	70	79
22	S	354/354 (100%)	351 (99%)	3 (1%)	73	80
23	U	161/161 (100%)	160 (99%)	1 (1%)	78	83
24	V	49/49 (100%)	48 (98%)	1 (2%)	48	66
25	W	66/66 (100%)	65 (98%)	1 (2%)	57	72
26	X	170/170 (100%)	169 (99%)	1 (1%)	78	83
27	Y	76/76 (100%)	76 (100%)	0	100	100
28	Z	130/130 (100%)	129 (99%)	1 (1%)	73	80
29	a	112/112 (100%)	112 (100%)	0	100	100
30	b	67/67 (100%)	65 (97%)	2 (3%)	36	57
31	c	187/187 (100%)	187 (100%)	0	100	100
32	d	17/17 (100%)	17 (100%)	0	100	100
33	e	114/114 (100%)	114 (100%)	0	100	100
34	f	174/174 (100%)	173 (99%)	1 (1%)	78	83
35	g	190/190 (100%)	190 (100%)	0	100	100
36	h	94/94 (100%)	94 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	i	196/196 (100%)	196 (100%)	0	100	100
38	j	106/106 (100%)	106 (100%)	0	100	100
39	k	87/87 (100%)	87 (100%)	0	100	100
40	l	57/57 (100%)	56 (98%)	1 (2%)	51	68
41	m	272/272 (100%)	272 (100%)	0	100	100
42	n	116/116 (100%)	116 (100%)	0	100	100
43	o	177/177 (100%)	176 (99%)	1 (1%)	78	83
44	p	64/64 (100%)	64 (100%)	0	100	100
45	q	207/207 (100%)	205 (99%)	2 (1%)	68	78
46	r	104/104 (100%)	101 (97%)	3 (3%)	37	58
47	s	113/113 (100%)	112 (99%)	1 (1%)	70	79
48	t	89/89 (100%)	89 (100%)	0	100	100
49	u	66/548 (12%)	63 (96%)	3 (4%)	24	46
50	w	360/928 (39%)	359 (100%)	1 (0%)	86	85
All	All	8396/10666 (79%)	8346 (99%)	50 (1%)	76	83

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	16	ASN
1	1	347	ILE
1	1	568	ILE
1	1	575	ILE
2	2	336	ILE
2	2	371	ILE
3	3	26	LEU
3	3	38	LEU
3	3	97	ASP
3	3	143	ASN
3	3	229	ARG
3	3	269	LYS
3	3	375	ILE
4	4	115	HIS
5	5	70	LEU
7	7	421	LEU
7	7	488	ILE
8	8	9	ILE

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Mol	Chain	Res	Type
8	8	221	ASP
9	9	517	LEU
12	G	8	ARG
17	L	89	ASP
17	L	98	VAL
19	P	19	VAL
19	P	115	VAL
19	P	265	LYS
21	R	28	LEU
22	S	228	VAL
22	S	284	VAL
22	S	309	VAL
23	U	165	ASN
24	V	120	VAL
25	W	48	VAL
26	X	122	LEU
28	Z	11	LEU
30	b	9	VAL
30	b	32	ILE
34	f	149	ASN
40	l	32	VAL
43	o	64	ASN
45	q	67	VAL
45	q	121	ILE
46	r	49	LEU
46	r	51	VAL
46	r	91	LEU
47	s	62	THR
49	u	12	VAL
49	u	13	THR
49	u	31	LEU
50	w	465	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (111) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	16	ASN
1	1	40	HIS
1	1	76	ASN
1	1	82	ASN
1	1	110	GLN
1	1	122	GLN

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Mol	Chain	Res	Type
1	1	159	GLN
1	1	180	GLN
1	1	207	GLN
1	1	212	HIS
1	1	221	ASN
1	1	270	GLN
1	1	274	ASN
1	1	288	ASN
1	1	301	HIS
1	1	309	ASN
1	1	372	ASN
1	1	442	GLN
1	1	477	HIS
1	1	481	GLN
1	1	512	GLN
1	1	551	GLN
1	1	586	ASN
2	2	355	GLN
2	2	377	ASN
2	2	386	ASN
2	2	487	GLN
2	2	610	ASN
2	2	716	HIS
2	2	753	HIS
2	2	758	ASN
3	3	12	HIS
3	3	17	HIS
3	3	49	ASN
3	3	80	GLN
3	3	138	GLN
3	3	143	ASN
3	3	180	GLN
3	3	224	ASN
3	3	231	ASN
3	3	247	GLN
3	3	264	ASN
3	3	302	ASN
3	3	309	GLN
3	3	321	ASN
3	3	335	ASN
3	3	354	ASN
3	3	361	ASN

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Mol	Chain	Res	Type
3	3	390	HIS
4	4	130	ASN
4	4	147	HIS
4	4	227	GLN
4	4	300	GLN
4	4	322	ASN
4	4	333	ASN
4	4	350	ASN
5	5	58	GLN
5	5	111	ASN
5	5	159	GLN
5	5	191	ASN
5	5	212	ASN
5	5	237	ASN
5	5	273	GLN
5	5	276	GLN
5	5	285	ASN
5	5	345	GLN
5	5	351	ASN
6	6	10	ASN
6	6	55	GLN
6	6	62	GLN
6	6	93	HIS
6	6	144	HIS
6	6	186	GLN
7	7	223	ASN
7	7	225	HIS
7	7	229	ASN
7	7	281	HIS
7	7	289	GLN
7	7	368	HIS
7	7	402	GLN
7	7	436	HIS
7	7	442	GLN
7	7	453	GLN
7	7	454	GLN
7	7	548	HIS
8	8	14	GLN
8	8	270	HIS
8	8	289	ASN
8	8	327	GLN
8	8	345	GLN

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Mol	Chain	Res	Type
8	8	346	GLN
8	8	355	ASN
8	8	359	GLN
9	9	236	HIS
9	9	303	ASN
9	9	376	ASN
9	9	399	GLN
9	9	448	GLN
9	9	456	GLN
9	9	479	GLN
9	9	480	GLN
49	u	37	ASN
50	w	208	GLN
50	w	224	ASN
50	w	414	ASN
50	w	446	ASN
50	w	500	ASN
50	w	522	GLN
50	w	578	HIS
50	w	595	GLN
50	w	598	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	1771/1776 (99%)	707 (39%)	51 (2%)
11	F	25/26 (96%)	14 (56%)	1 (4%)
18	N	74/75 (98%)	21 (28%)	2 (2%)
All	All	1870/1877 (99%)	742 (39%)	54 (2%)

All (742) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
10	A	3	C
10	A	4	C
10	A	9	U
10	A	17	C
10	A	20	G
10	A	25	A
10	A	26	U
10	A	33	G

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Mol	Chain	Res	Type
10	A	37	C
10	A	41	G
10	A	42	A
10	A	44	U
10	A	46	A
10	A	49	C
10	A	53	C
10	A	55	U
10	A	56	G
10	A	60	A
10	A	62	G
10	A	65	C
10	A	66	G
10	A	67	C
10	A	68	A
10	A	72	C
10	A	73	C
10	A	75	G
10	A	76	U
10	A	77	A
10	A	78	C
10	A	79	A
10	A	80	G
10	A	81	U
10	A	84	A
10	A	92	A
10	A	99	A
10	A	103	A
10	A	113	G
10	A	114	G
10	A	115	U
10	A	125	C
10	A	126	G
10	A	127	C
10	A	128	U
10	A	129	C
10	A	130	G
10	A	131	C
10	A	132	U
10	A	133	C
10	A	134	C
10	A	135	U

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Mol	Chain	Res	Type
10	A	136	C
10	A	137	U
10	A	139	C
10	A	140	U
10	A	141	A
10	A	142	C
10	A	143	U
10	A	146	G
10	A	147	A
10	A	148	U
10	A	155	G
10	A	160	U
10	A	161	U
10	A	164	A
10	A	168	C
10	A	170	A
10	A	171	A
10	A	172	U
10	A	176	U
10	A	178	C
10	A	179	C
10	A	182	C
10	A	183	G
10	A	184	G
10	A	186	G
10	A	187	C
10	A	188	U
10	A	189	G
10	A	190	A
10	A	191	C
10	A	196	U
10	A	197	U
10	A	198	U
10	A	199	G
10	A	200	U
10	A	203	G
10	A	204	G
10	A	208	G
10	A	212	G
10	A	219	U
10	A	220	C
10	A	223	A

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Mol	Chain	Res	Type
10	A	224	U
10	A	225	C
10	A	226	A
10	A	228	A
10	A	232	A
10	A	234	C
10	A	235	C
10	A	239	U
10	A	240	C
10	A	241	A
10	A	269	C
10	A	270	G
10	A	272	C
10	A	273	G
10	A	275	C
10	A	276	U
10	A	277	U
10	A	278	U
10	A	279	G
10	A	286	C
10	A	289	G
10	A	293	A
10	A	295	C
10	A	296	U
10	A	297	C
10	A	300	G
10	A	303	G
10	A	304	A
10	A	305	U
10	A	307	G
10	A	311	C
10	A	313	C
10	A	314	U
10	A	315	C
10	A	316	C
10	A	318	U
10	A	321	C
10	A	322	G
10	A	326	A
10	A	331	C
10	A	332	C
10	A	335	U

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Mol	Chain	Res	Type
10	A	337	G
10	A	340	C
10	A	346	C
10	A	351	U
10	A	352	C
10	A	354	A
10	A	357	U
10	A	358	U
10	A	359	C
10	A	360	G
10	A	362	U
10	A	365	U
10	A	374	U
10	A	375	G
10	A	376	C
10	A	379	A
10	A	382	A
10	A	383	U
10	A	388	A
10	A	390	C
10	A	398	A
10	A	399	C
10	A	403	G
10	A	411	G
10	A	413	U
10	A	416	A
10	A	418	U
10	A	428	G
10	A	433	U
10	A	438	A
10	A	440	C
10	A	441	G
10	A	442	G
10	A	454	A
10	A	455	A
10	A	456	G
10	A	457	G
10	A	461	G
10	A	462	C
10	A	463	A
10	A	464	G
10	A	466	A

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Mol	Chain	Res	Type
10	A	470	G
10	A	472	G
10	A	473	C
10	A	474	A
10	A	477	U
10	A	478	U
10	A	480	C
10	A	481	C
10	A	482	C
10	A	486	C
10	A	490	A
10	A	491	C
10	A	496	G
10	A	497	G
10	A	500	G
10	A	502	A
10	A	503	G
10	A	505	G
10	A	506	A
10	A	511	A
10	A	513	A
10	A	515	A
10	A	516	A
10	A	518	A
10	A	519	A
10	A	520	U
10	A	522	C
10	A	523	A
10	A	524	G
10	A	525	G
10	A	526	A
10	A	527	C
10	A	528	U
10	A	532	U
10	A	538	C
10	A	540	C
10	A	541	U
10	A	543	U
10	A	545	A
10	A	546	U
10	A	547	U
10	A	548	G

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Mol	Chain	Res	Type
10	A	549	G
10	A	550	A
10	A	551	A
10	A	553	G
10	A	554	A
10	A	558	C
10	A	560	C
10	A	562	U
10	A	564	A
10	A	566	A
10	A	572	U
10	A	575	C
10	A	576	G
10	A	578	G
10	A	580	A
10	A	581	U
10	A	582	C
10	A	583	C
10	A	584	A
10	A	590	G
10	A	594	A
10	A	595	A
10	A	596	G
10	A	598	C
10	A	599	U
10	A	602	U
10	A	603	C
10	A	604	G
10	A	607	G
10	A	609	A
10	A	613	G
10	A	616	G
10	A	617	U
10	A	619	A
10	A	620	U
10	A	621	U
10	A	622	C
10	A	623	C
10	A	624	A
10	A	633	A
10	A	634	G
10	A	640	A

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Mol	Chain	Res	Type
10	A	643	A
10	A	646	G
10	A	653	C
10	A	658	A
10	A	659	A
10	A	660	A
10	A	661	A
10	A	662	A
10	A	663	G
10	A	678	U
10	A	679	U
10	A	731	C
10	A	734	C
10	A	735	C
10	A	736	C
10	A	745	U
10	A	746	C
10	A	749	C
10	A	755	C
10	A	756	U
10	A	757	C
10	A	758	G
10	A	759	A
10	A	776	U
10	A	777	C
10	A	780	G
10	A	781	C
10	A	782	G
10	A	784	G
10	A	785	G
10	A	788	C
10	A	789	G
10	A	790	A
10	A	792	G
10	A	793	C
10	A	794	G
10	A	795	U
10	A	797	U
10	A	803	G
10	A	804	A
10	A	807	A
10	A	808	A

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Mol	Chain	Res	Type
10	A	811	U
10	A	818	U
10	A	822	A
10	A	826	A
10	A	827	G
10	A	830	C
10	A	833	A
10	A	835	C
10	A	836	C
10	A	837	G
10	A	841	G
10	A	843	A
10	A	844	U
10	A	846	C
10	A	847	C
10	A	848	G
10	A	849	C
10	A	852	C
10	A	853	U
10	A	857	A
10	A	864	G
10	A	865	A
10	A	866	A
10	A	868	A
10	A	869	G
10	A	871	A
10	A	873	C
10	A	874	G
10	A	875	C
10	A	877	G
10	A	879	U
10	A	883	U
10	A	884	U
10	A	886	U
10	A	894	U
10	A	897	G
10	A	899	A
10	A	902	U
10	A	903	G
10	A	904	A
10	A	905	G
10	A	906	G

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Mol	Chain	Res	Type
10	A	907	C
10	A	908	C
10	A	909	A
10	A	910	U
10	A	913	U
10	A	915	A
10	A	916	A
10	A	917	G
10	A	924	G
10	A	926	C
10	A	929	G
10	A	933	C
10	A	939	U
10	A	941	U
10	A	947	C
10	A	949	C
10	A	950	U
10	A	951	A
10	A	957	G
10	A	963	C
10	A	964	U
10	A	965	U
10	A	966	G
10	A	967	G
10	A	969	C
10	A	971	G
10	A	973	C
10	A	977	A
10	A	982	G
10	A	986	A
10	A	988	A
10	A	995	G
10	A	997	A
10	A	999	U
10	A	1002	C
10	A	1006	G
10	A	1012	U
10	A	1013	U
10	A	1016	A
10	A	1019	A
10	A	1027	A
10	A	1028	C

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Mol	Chain	Res	Type
10	A	1034	U
10	A	1035	C
10	A	1038	A
10	A	1041	U
10	A	1043	C
10	A	1045	A
10	A	1046	A
10	A	1047	G
10	A	1049	C
10	A	1050	G
10	A	1056	A
10	A	1057	U
10	A	1058	A
10	A	1062	U
10	A	1065	U
10	A	1070	C
10	A	1074	C
10	A	1076	A
10	A	1079	A
10	A	1080	A
10	A	1081	C
10	A	1082	G
10	A	1083	A
10	A	1084	U
10	A	1093	G
10	A	1100	G
10	A	1105	C
10	A	1106	G
10	A	1110	U
10	A	1111	U
10	A	1113	C
10	A	1114	C
10	A	1116	U
10	A	1125	G
10	A	1126	G
10	A	1127	G
10	A	1129	A
10	A	1133	U
10	A	1134	C
10	A	1135	C
10	A	1136	G
10	A	1139	A

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Mol	Chain	Res	Type
10	A	1142	C
10	A	1144	A
10	A	1147	G
10	A	1149	C
10	A	1150	U
10	A	1151	U
10	A	1155	G
10	A	1157	U
10	A	1175	G
10	A	1179	A
10	A	1190	A
10	A	1194	G
10	A	1199	G
10	A	1200	A
10	A	1202	G
10	A	1205	A
10	A	1208	G
10	A	1211	C
10	A	1212	C
10	A	1213	A
10	A	1217	G
10	A	1220	G
10	A	1225	G
10	A	1236	A
10	A	1238	U
10	A	1239	U
10	A	1247	A
10	A	1248	C
10	A	1249	A
10	A	1250	C
10	A	1252	G
10	A	1253	G
10	A	1255	A
10	A	1258	C
10	A	1270	G
10	A	1271	G
10	A	1272	A
10	A	1279	C
10	A	1280	A
10	A	1281	G
10	A	1288	C
10	A	1289	A

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Mol	Chain	Res	Type
10	A	1294	G
10	A	1297	A
10	A	1298	G
10	A	1299	C
10	A	1300	U
10	A	1302	U
10	A	1303	U
10	A	1304	U
10	A	1305	C
10	A	1307	C
10	A	1309	A
10	A	1311	U
10	A	1312	C
10	A	1317	G
10	A	1322	U
10	A	1326	G
10	A	1327	C
10	A	1329	U
10	A	1330	G
10	A	1339	U
10	A	1343	U
10	A	1353	A
10	A	1354	U
10	A	1360	U
10	A	1365	A
10	A	1367	U
10	A	1368	U
10	A	1369	C
10	A	1374	A
10	A	1378	A
10	A	1382	A
10	A	1386	U
10	A	1391	C
10	A	1392	A
10	A	1393	U
10	A	1394	G
10	A	1397	A
10	A	1398	A
10	A	1400	U
10	A	1402	G
10	A	1406	C
10	A	1407	G

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Mol	Chain	Res	Type
10	A	1408	C
10	A	1409	G
10	A	1413	C
10	A	1414	C
10	A	1415	C
10	A	1420	G
10	A	1421	G
10	A	1424	G
10	A	1426	C
10	A	1428	U
10	A	1431	C
10	A	1432	C
10	A	1433	C
10	A	1434	A
10	A	1437	U
10	A	1442	A
10	A	1445	G
10	A	1448	A
10	A	1450	A
10	A	1451	A
10	A	1452	G
10	A	1454	G
10	A	1458	U
10	A	1459	U
10	A	1462	G
10	A	1470	A
10	A	1471	G
10	A	1472	A
10	A	1476	A
10	A	1484	C
10	A	1485	A
10	A	1486	G
10	A	1487	G
10	A	1489	C
10	A	1490	U
10	A	1491	G
10	A	1493	G
10	A	1494	A
10	A	1495	U
10	A	1498	C
10	A	1499	C
10	A	1502	A

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Mol	Chain	Res	Type
10	A	1503	G
10	A	1504	A
10	A	1505	U
10	A	1506	G
10	A	1507	U
10	A	1509	G
10	A	1514	U
10	A	1515	G
10	A	1516	C
10	A	1526	A
10	A	1527	C
10	A	1531	G
10	A	1535	G
10	A	1537	C
10	A	1539	C
10	A	1540	A
10	A	1543	G
10	A	1545	G
10	A	1548	C
10	A	1550	U
10	A	1551	A
10	A	1552	C
10	A	1553	C
10	A	1555	U
10	A	1562	G
10	A	1565	G
10	A	1567	C
10	A	1568	G
10	A	1569	C
10	A	1572	G
10	A	1574	A
10	A	1575	A
10	A	1576	C
10	A	1581	U
10	A	1582	G
10	A	1583	A
10	A	1587	C
10	A	1590	U
10	A	1591	U
10	A	1594	U
10	A	1595	G
10	A	1596	A

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Mol	Chain	Res	Type
10	A	1597	U
10	A	1598	G
10	A	1599	G
10	A	1601	G
10	A	1609	A
10	A	1614	A
10	A	1617	U
10	A	1618	A
10	A	1624	C
10	A	1625	A
10	A	1632	A
10	A	1633	G
10	A	1636	A
10	A	1638	U
10	A	1643	G
10	A	1649	G
10	A	1655	C
10	A	1659	A
10	A	1660	G
10	A	1665	C
10	A	1666	G
10	A	1670	A
10	A	1674	A
10	A	1675	G
10	A	1683	C
10	A	1684	C
10	A	1685	U
10	A	1686	U
10	A	1690	A
10	A	1691	C
10	A	1694	A
10	A	1695	C
10	A	1696	C
10	A	1697	G
10	A	1698	C
10	A	1699	C
10	A	1700	C
10	A	1710	A
10	A	1712	C
10	A	1716	U
10	A	1717	G
10	A	1724	U

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Mol	Chain	Res	Type
10	A	1728	U
10	A	1730	A
10	A	1732	G
10	A	1733	C
10	A	1734	C
10	A	1737	C
10	A	1738	G
10	A	1739	G
10	A	1740	A
10	A	1741	U
10	A	1743	G
10	A	1746	C
10	A	1747	C
10	A	1748	G
10	A	1749	C
10	A	1751	G
10	A	1757	G
10	A	1760	C
10	A	1761	C
10	A	1762	A
10	A	1763	C
10	A	1776	G
10	A	1777	C
10	A	1778	G
10	A	1779	C
10	A	1780	U
10	A	1781	G
10	A	1782	A
10	A	1784	A
10	A	1787	A
10	A	1788	C
10	A	1790	G
10	A	1791	U
10	A	1792	C
10	A	1793	G
10	A	1795	A
10	A	1797	U
10	A	1798	U
10	A	1799	G
10	A	1801	C
10	A	1803	A
10	A	1804	U

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Mol	Chain	Res	Type
10	A	1808	G
10	A	1809	A
10	A	1810	G
10	A	1813	A
10	A	1817	A
10	A	1818	A
10	A	1819	A
10	A	1820	G
10	A	1825	A
10	A	1826	A
10	A	1829	A
10	A	1830	G
10	A	1832	U
10	A	1833	U
10	A	1837	G
10	A	1838	U
10	A	1843	G
10	A	1846	C
10	A	1852	G
10	A	1853	A
10	A	1855	G
10	A	1857	A
10	A	1858	U
10	A	1859	C
10	A	1860	A
10	A	1861	U
10	A	1863	A
11	F	4	A
11	F	6	A
11	F	8	A
11	F	9	C
11	F	10	C
11	F	14	G
11	F	17	C
11	F	18	A
11	F	19	C
11	F	23	A
11	F	24	C
11	F	25	U
11	F	26	C
11	F	27	C
18	N	8	U

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Mol	Chain	Res	Type
18	N	9	G
18	N	16	C
18	N	17	G
18	N	19	A
18	N	20	A
18	N	21	G
18	N	23	G
18	N	29	G
18	N	33	C
18	N	34	A
18	N	46	U
18	N	47	C
18	N	48	G
18	N	51	G
18	N	54	U
18	N	58	A
18	N	62	A
18	N	72	A
18	N	73	C
18	N	74	C

All (54) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
10	A	2	A
10	A	24	C
10	A	65	C
10	A	66	G
10	A	102	A
10	A	127	C
10	A	131	C
10	A	133	C
10	A	138	C
10	A	140	U
10	A	141	A
10	A	189	G
10	A	222	G
10	A	225	C
10	A	278	U
10	A	285	U
10	A	317	G
10	A	455	A

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Mol	Chain	Res	Type
10	A	521	A
10	A	522	C
10	A	524	G
10	A	540	C
10	A	542	G
10	A	594	A
10	A	619	A
10	A	730	C
10	A	817	G
10	A	829	C
10	A	865	A
10	A	876	G
10	A	1133	U
10	A	1249	A
10	A	1279	C
10	A	1303	U
10	A	1390	G
10	A	1391	C
10	A	1392	A
10	A	1397	A
10	A	1412	C
10	A	1414	C
10	A	1425	G
10	A	1490	U
10	A	1538	U
10	A	1594	U
10	A	1632	A
10	A	1674	A
10	A	1716	U
10	A	1750	C
10	A	1817	A
10	A	1819	A
10	A	1824	U
11	F	8	A
18	N	45	G
18	N	73	C

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
10	A	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	736:C	O3'	744:C	P	27.46
1	A	761:G	O3'	774:U	P	18.00
1	A	679:U	O3'	683:G	P	15.42
1	A	687:G	O3'	730:C	P	13.04
1	A	243:C	O3'	267:G	P	13.01

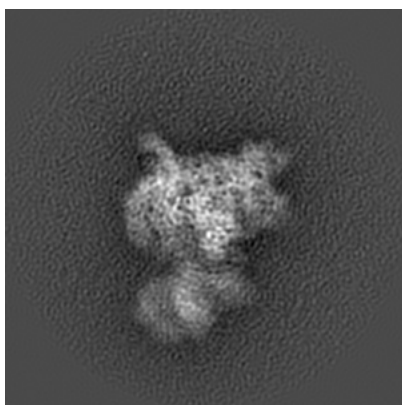
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4242. These allow visual inspection of the internal detail of the map and identification of artifacts.

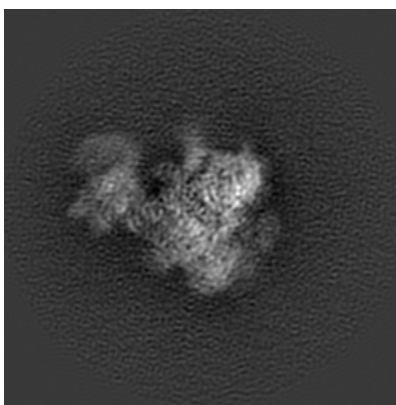
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

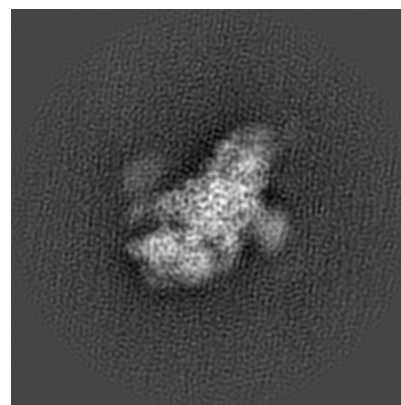
6.1.1 Primary map



X



Y

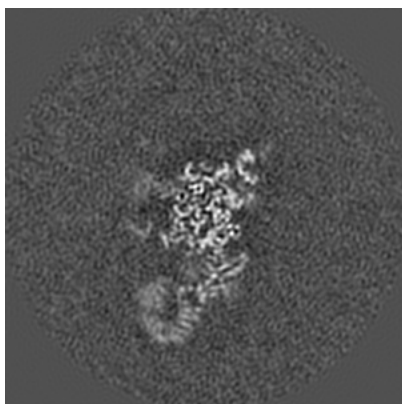


Z

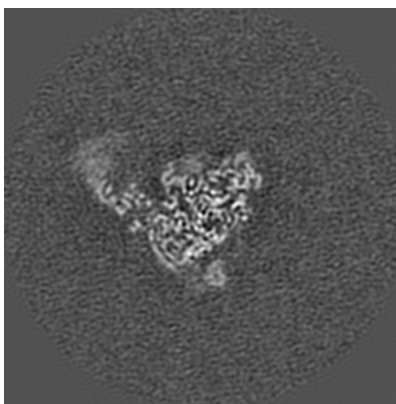
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

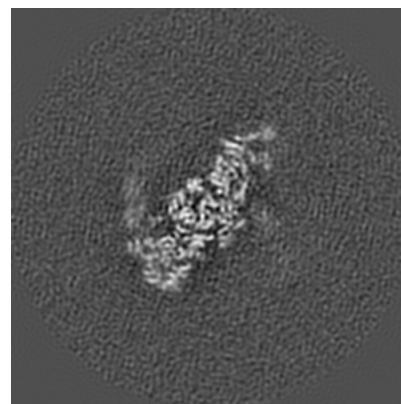
6.2.1 Primary map



X Index: 104



Y Index: 104

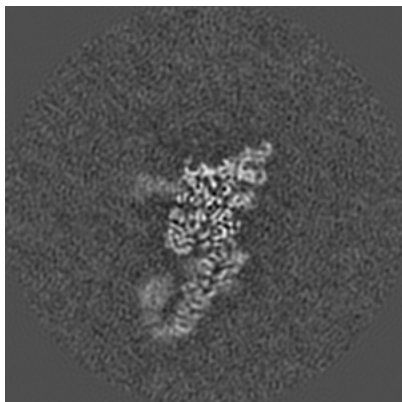


Z Index: 104

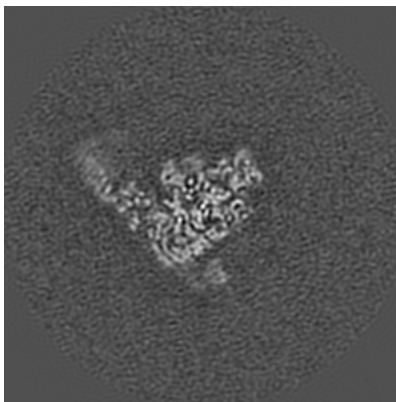
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

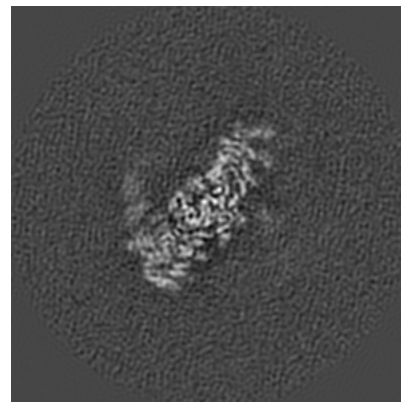
6.3.1 Primary map



X Index: 106



Y Index: 105

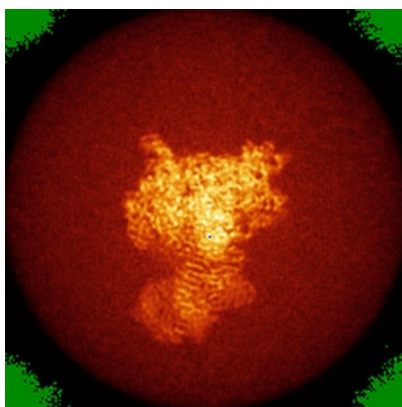


Z Index: 105

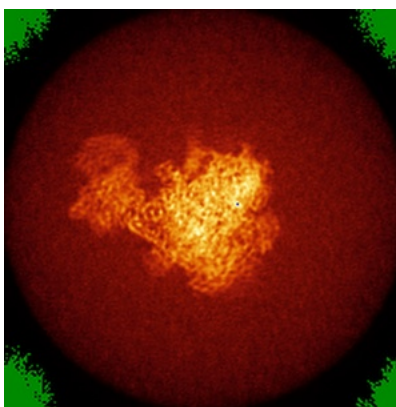
The images above show the largest variance slices of the map in three orthogonal directions.

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

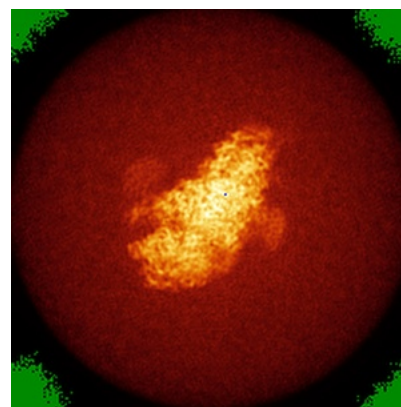
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

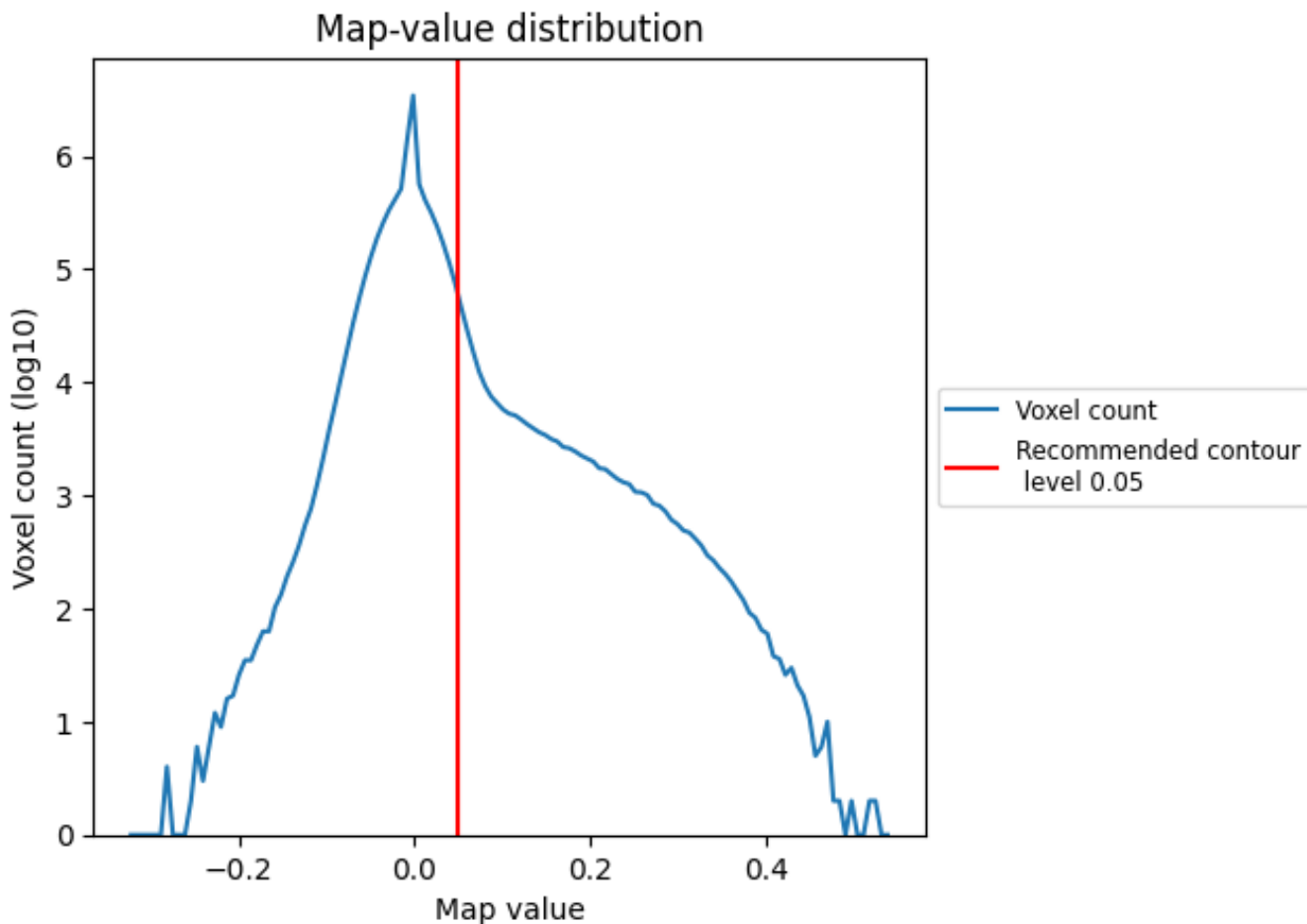
6.6 Mask visualisation

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

7 Map analysis [i](#)

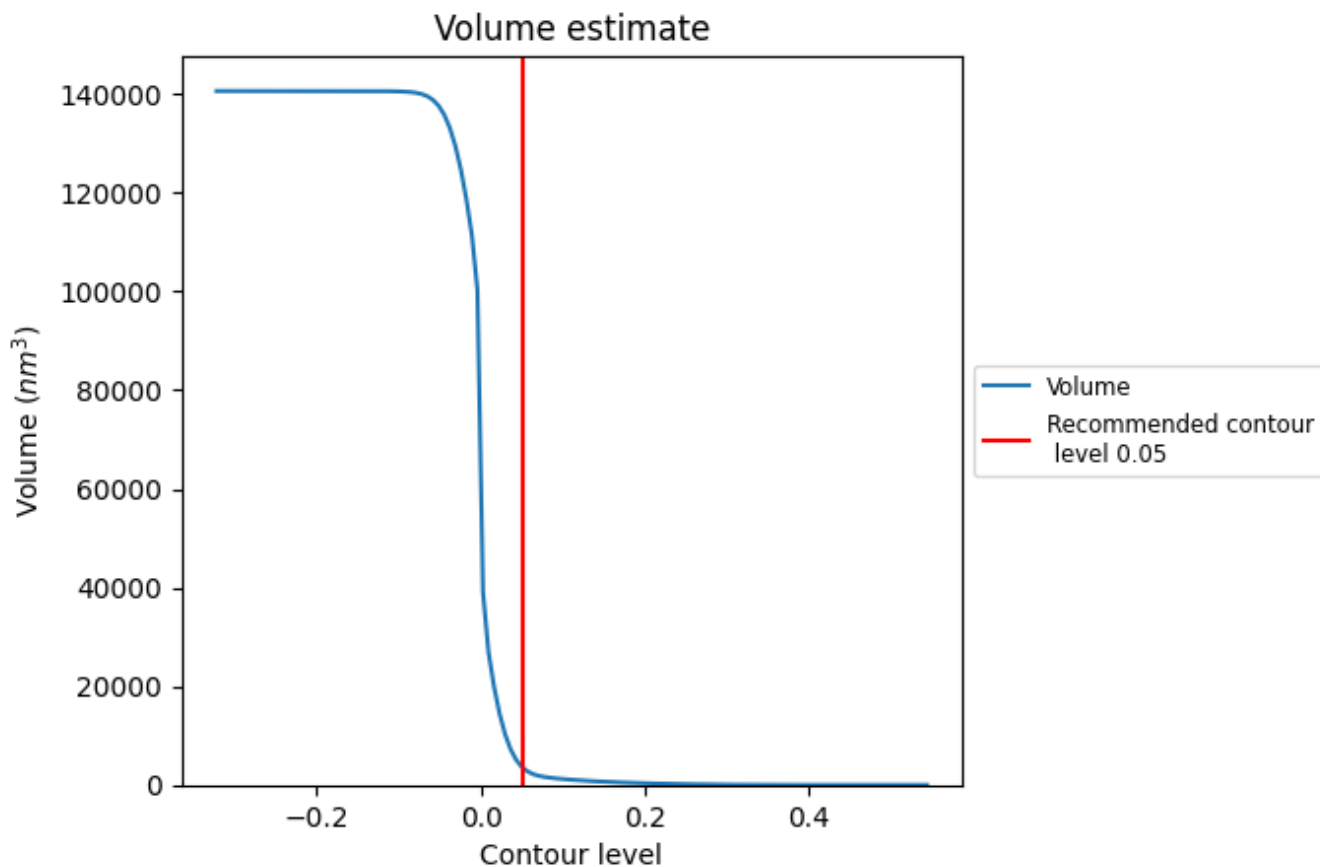
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

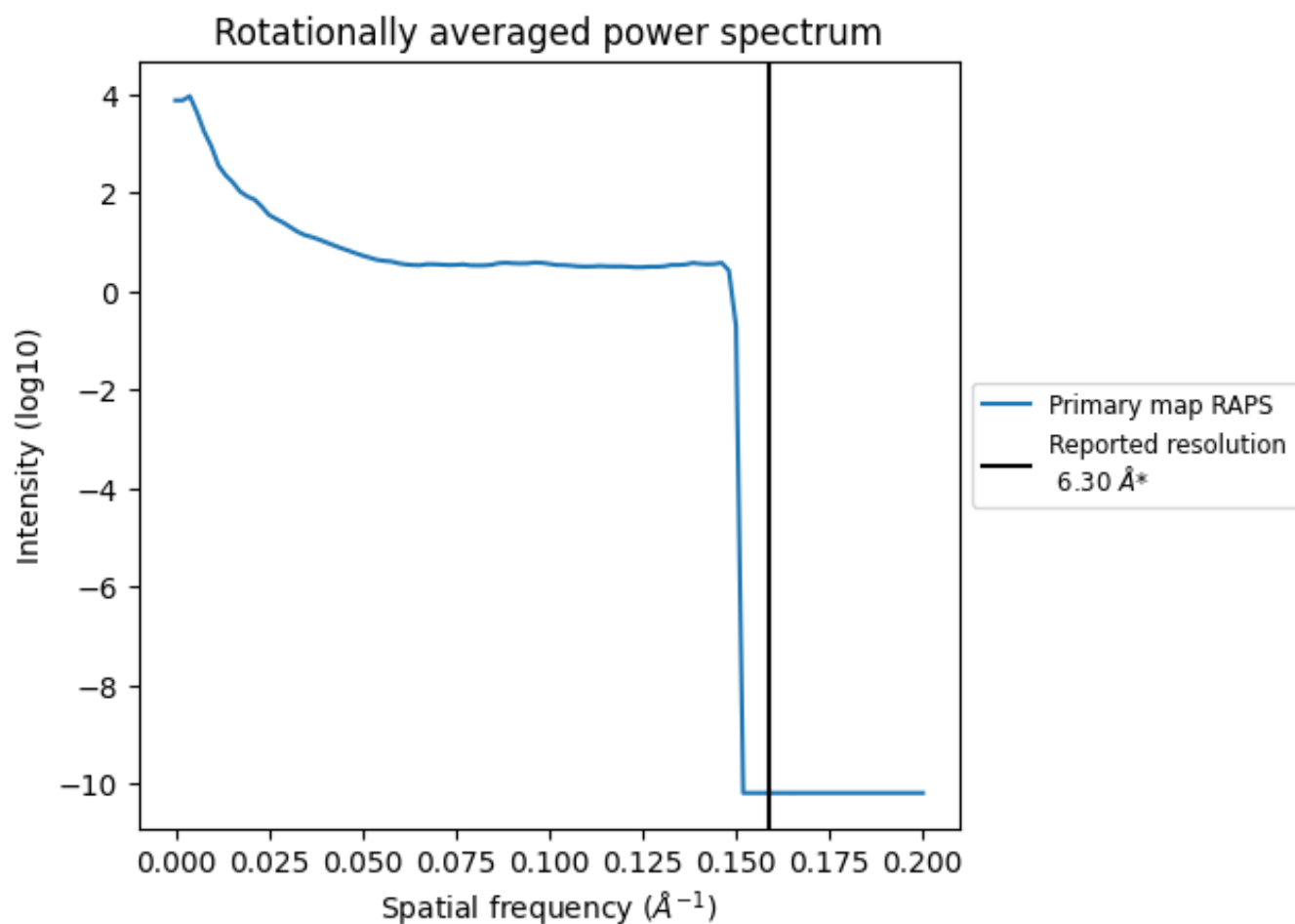
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 3639 nm^3 ; this corresponds to an approximate mass of 3287 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.159 Å⁻¹

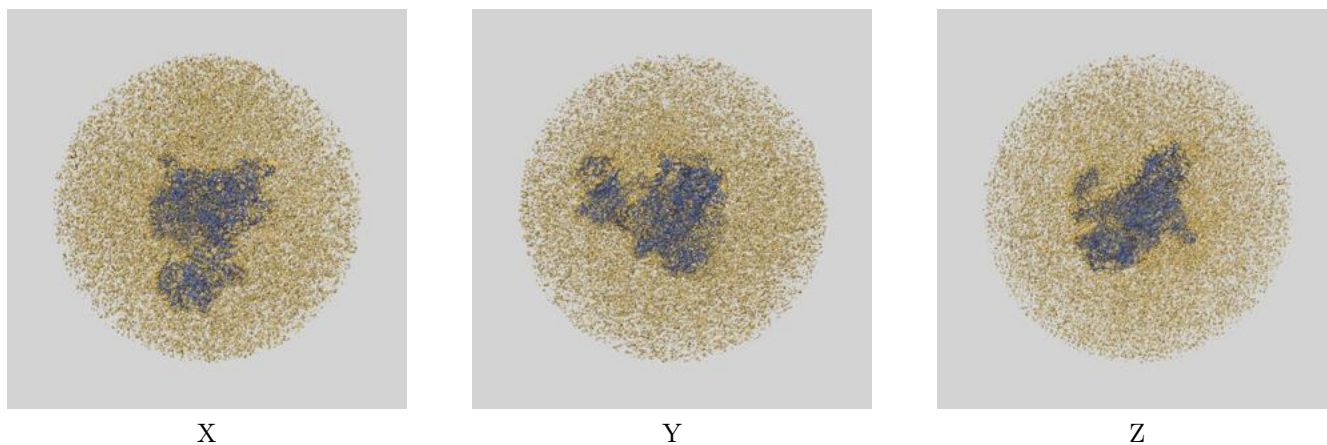
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

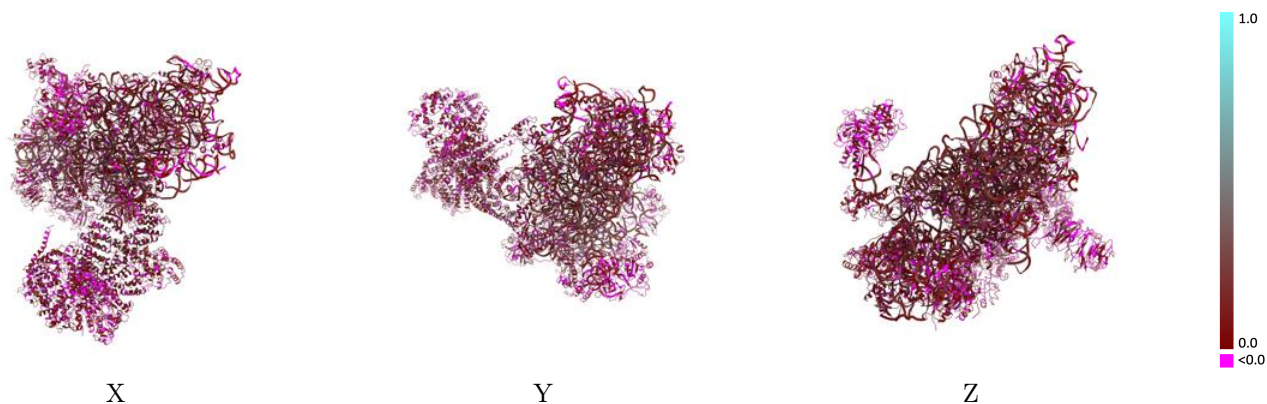
This section contains information regarding the fit between EMDB map EMD-4242 and PDB model 6FEC. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.05 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](#)

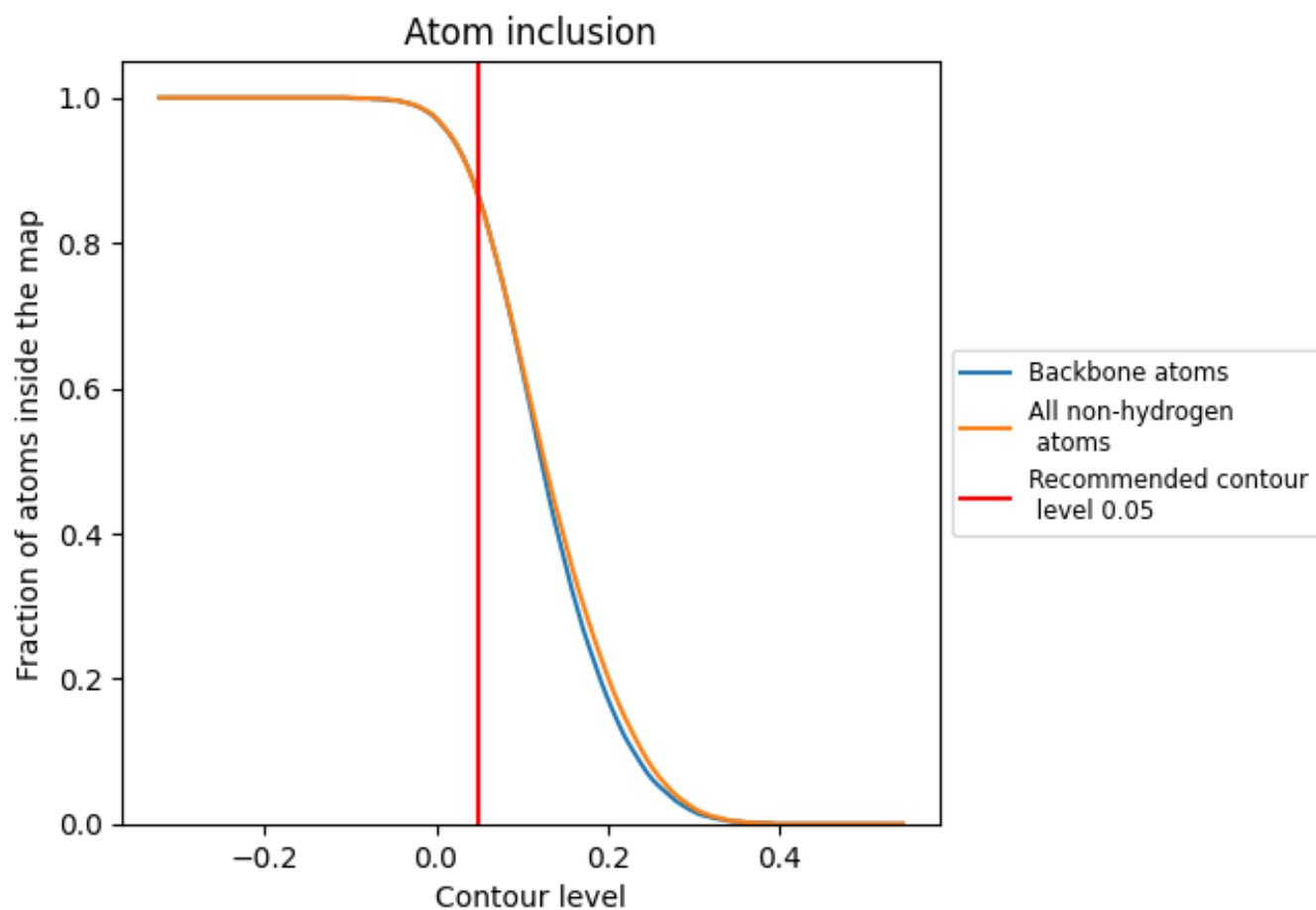


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 86% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8620	 0.1160
1	 0.8530	 0.1170
2	 0.8640	 0.1310
3	 0.9130	 0.1020
4	 0.8980	 0.0660
5	 0.8600	 0.0680
6	 0.9220	 0.0560
7	 0.9060	 0.0550
8	 0.9230	 0.0780
9	 0.7720	 0.0900
A	 0.9710	 0.1650
F	 0.7450	 0.0990
G	 0.8160	 0.0920
H	 0.8390	 0.1000
I	 0.8350	 0.1160
J	 0.7610	 0.0440
K	 0.8010	 0.1050
L	 0.8720	 0.0990
N	 0.9210	 0.1350
P	 0.6210	 0.0750
Q	 0.8130	 0.1090
R	 0.8920	 0.0970
S	 0.6430	 0.0230
U	 0.8020	 0.1000
V	 0.8470	 0.0780
W	 0.8800	 0.1020
X	 0.8270	 0.1240
Y	 0.8080	 0.1290
Z	 0.8070	 0.1180
a	 0.7810	 0.1230
b	 0.8150	 0.1160
c	 0.7990	 0.1310
d	 0.6500	 0.0460
e	 0.7810	 0.1090
f	 0.8350	 0.1230



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Chain	Atom inclusion	Q-score
g	 0.8240	 0.1140
h	 0.8400	 0.0840
i	 0.8430	 0.1250
j	 0.8160	 0.0780
k	 0.7790	 0.1050
l	 0.8090	 0.1020
m	 0.8980	 0.1010
n	 0.8480	 0.0800
o	 0.8740	 0.0940
p	 0.8520	 0.0550
q	 0.8850	 0.0850
r	 0.8960	 0.0800
s	 0.8590	 0.0990
t	 0.8500	 0.1060
u	 0.7870	 0.0800
w	 0.2680	 0.0140