



Full wwPDB EM Validation Report ⓘ

Oct 6, 2024 – 04:13 am BST

PDB ID : 6FEC
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:

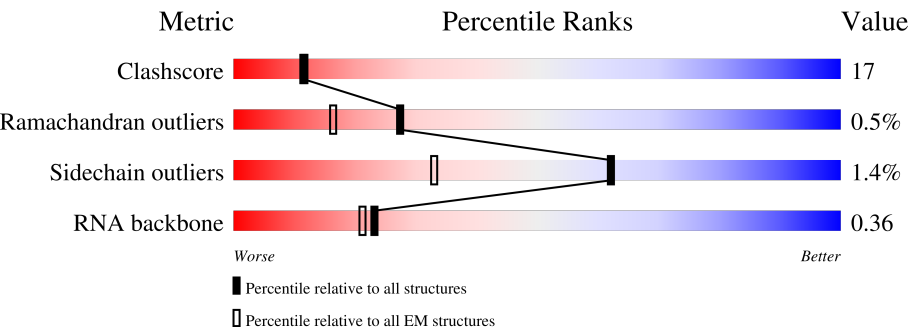
EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

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.






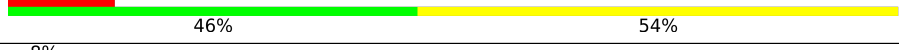
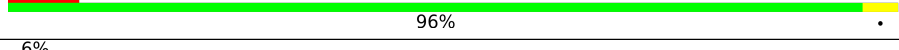
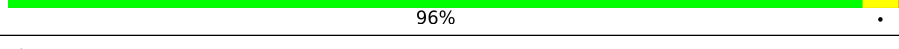
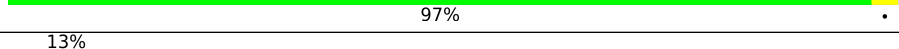
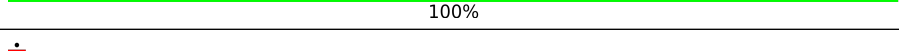
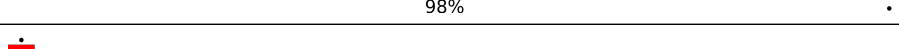
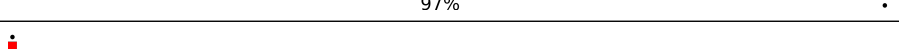
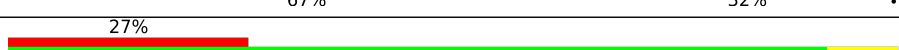
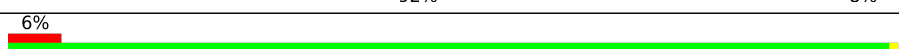
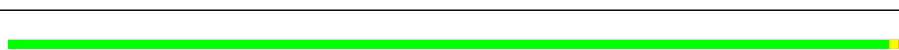
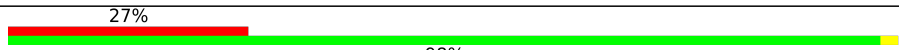
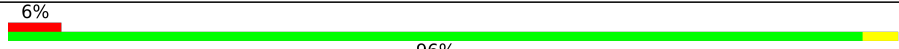


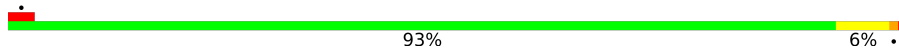
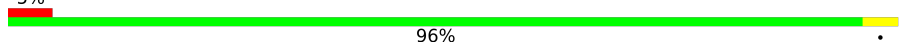
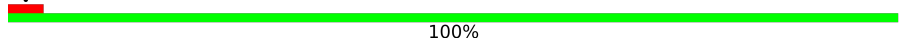
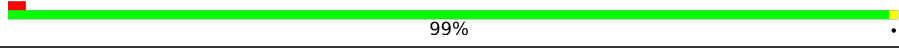
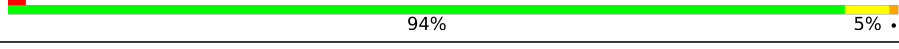
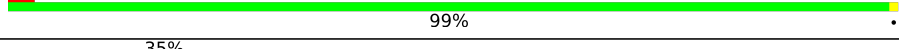
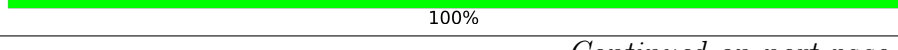

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	1	1362	<div><div>23%</div><div>20%</div><div>•</div><div>56%</div></div>
2	2	843	<div><div>40%</div><div>25%</div><div>•</div><div>34%</div></div>
3	3	445	<div><div>54%</div><div>38%</div><div>•</div><div>6%</div></div>
4	4	364	<div><div>39%</div><div>34%</div><div>•</div><div>25%</div></div>
5	5	352	<div><div>7%</div><div>56%</div><div>34%</div><div>•</div><div>8%</div></div>
6	6	218	<div><div>59%</div><div>40%</div><div>•</div></div>
7	7	564	<div><div>44%</div><div>22%</div><div>•</div><div>34%</div></div>

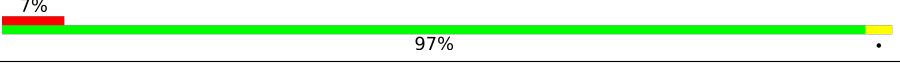
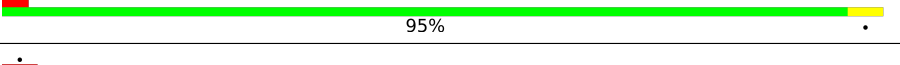
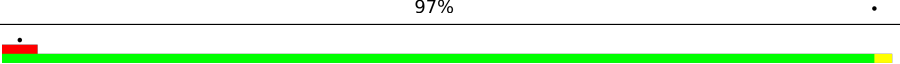
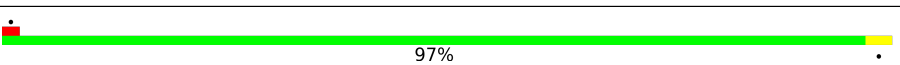
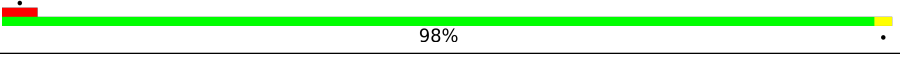
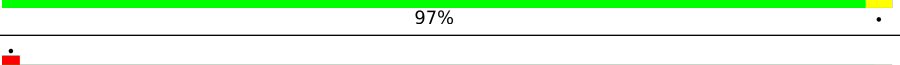
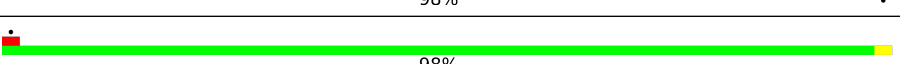
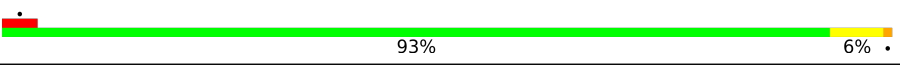
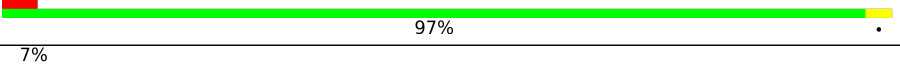

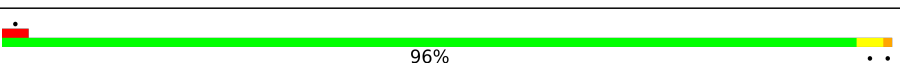
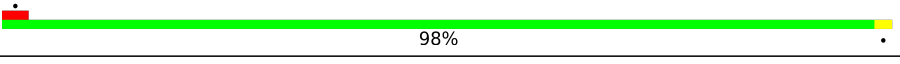
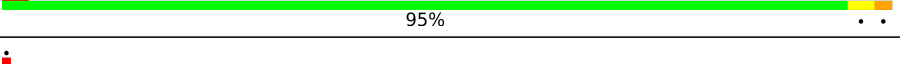





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Mol	Chain	Length	Quality of chain
8	8	374	
9	9	368	
10	A	1776	
11	F	26	
12	G	158	
13	H	141	
14	I	263	
15	J	53	
16	K	182	
17	L	137	
18	N	75	
19	P	266	
20	Q	142	
21	R	141	
22	S	422	
23	U	191	
24	V	59	
25	W	75	
26	X	190	
27	Y	84	
28	Z	150	
29	a	129	
30	b	82	
31	c	226	
32	d	17	

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Mol	Chain	Length	Quality of chain
33	e	126	
34	f	208	
35	g	227	
36	h	104	
37	i	215	
38	j	136	
39	k	99	
40	l	64	
41	m	313	
42	n	127	
43	o	206	
44	p	71	
45	q	237	
46	r	124	
47	s	131	
48	t	98	
49	u	636	
50	w	1121	

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
1	1	600	Total	C	N	O	S	0	1
			4935	3107	893	914	21		

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

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

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

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

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

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

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

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

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

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

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
7	7	373	Total	C	N	O	S	0	1
			3110	2010	520	563	17		

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
8	8	366	Total	C	N	O	S	0	1
			2919	1850	494	558	17		

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

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

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

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

- 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
24	V	59	Total	C	N	O	S	0	0
			473	293	104	75	1		

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
25	W	75	Total	C	N	O	S	0	0
			599	382	111	105	1		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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
36	h	104	Total	C	N	O	S	0	0
			822	514	156	148	4		

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

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

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
38	j	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

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

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

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

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

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

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

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

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

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
43	o	206	Total	C	N	O	S	0	0
			1680	1054	329	292	5		

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
44	p	71	Total	C	N	O	S	0	0
			582	367	109	99	7		

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

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

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

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

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

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

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
48	t	98	Total	C	N	O	S	0	0
			828	539	148	135	6		

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

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

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
50	w	403	Total	C	N	O	S	0	0
			3308	2132	573	587	16		

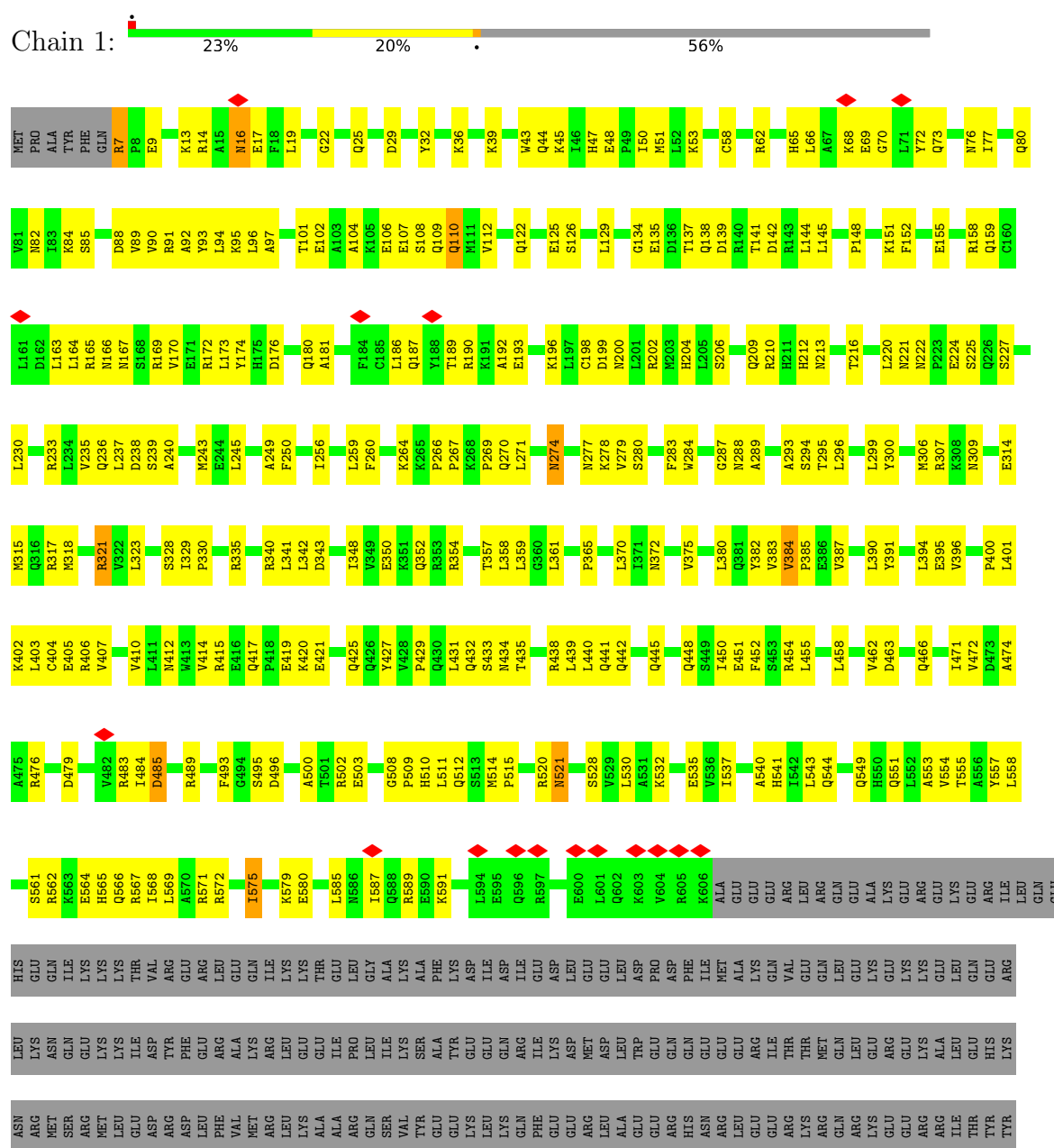
- Molecule 51 is water.

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

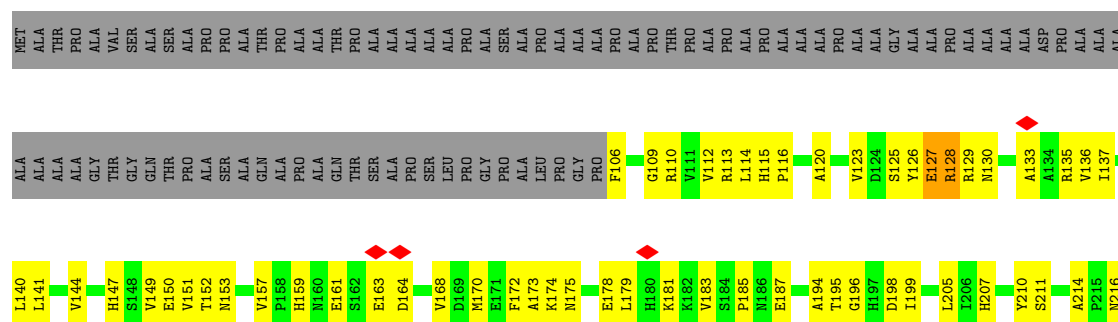
3 Residue-property plots

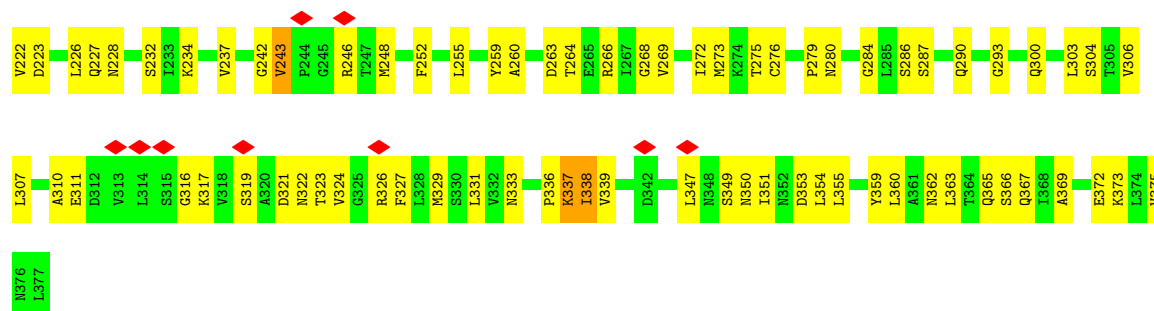
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Eukaryotic translation initiation factor 3 subunit A

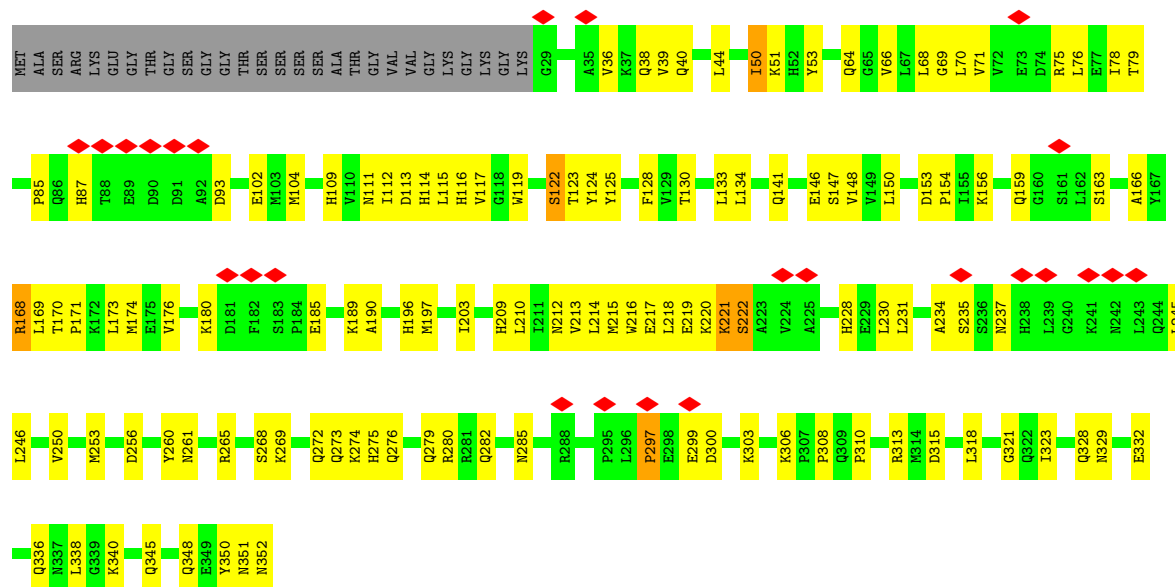




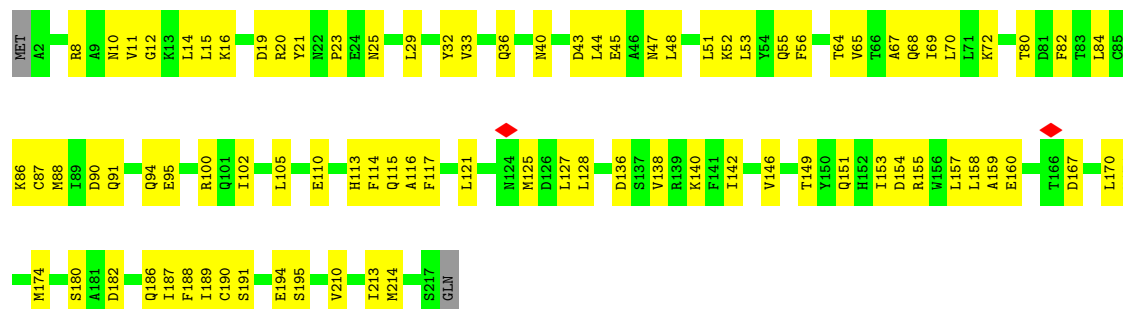




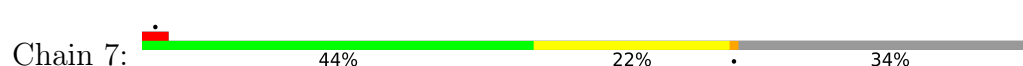
- Molecule 5: Eukaryotic translation initiation factor 3 subunit H

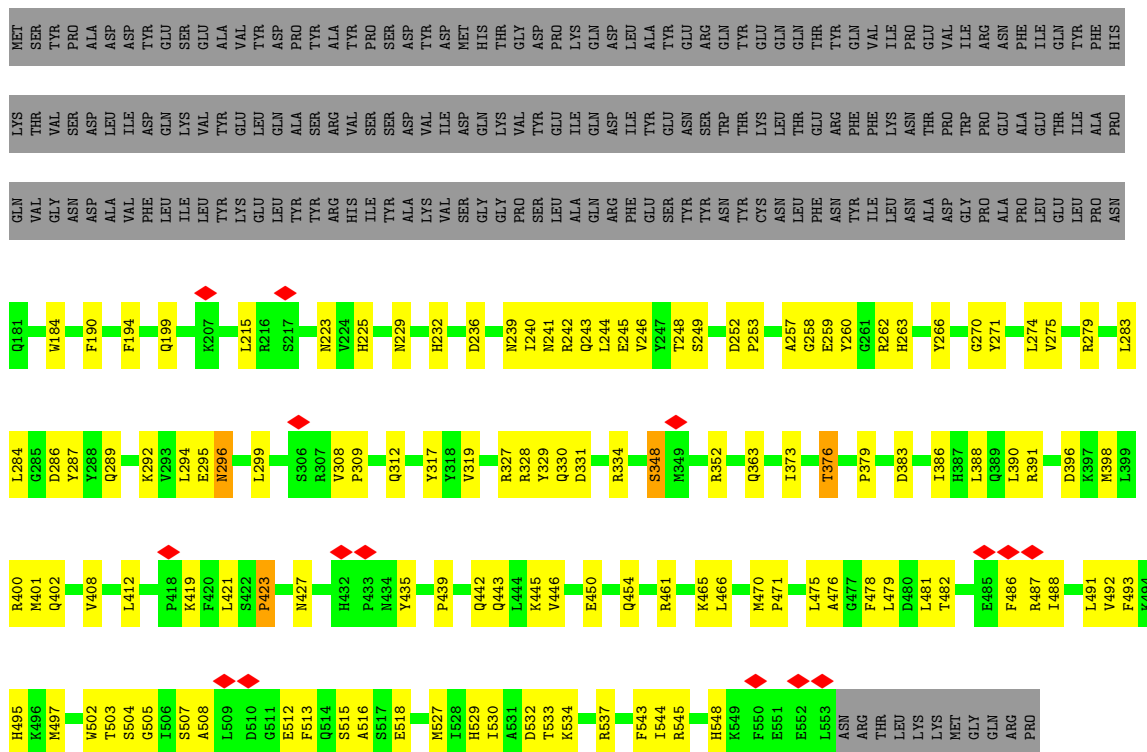


- Molecule 6: Eukaryotic translation initiation factor 3 subunit K

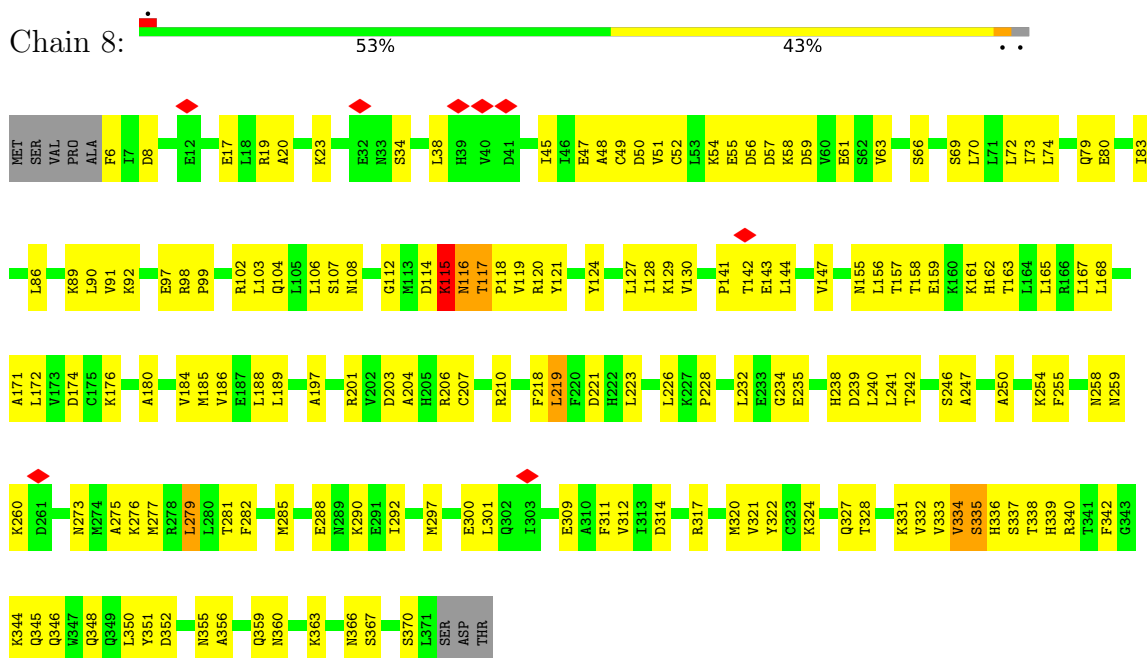


- Molecule 7: Eukaryotic translation initiation factor 3 subunit L

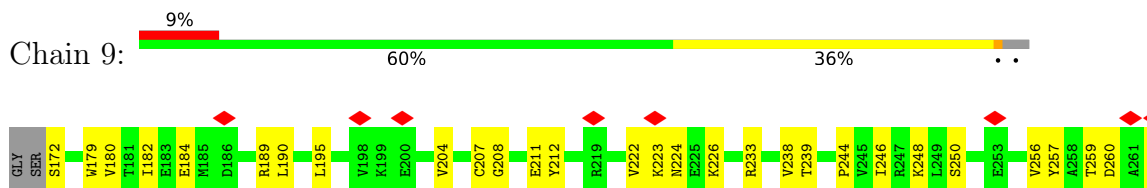


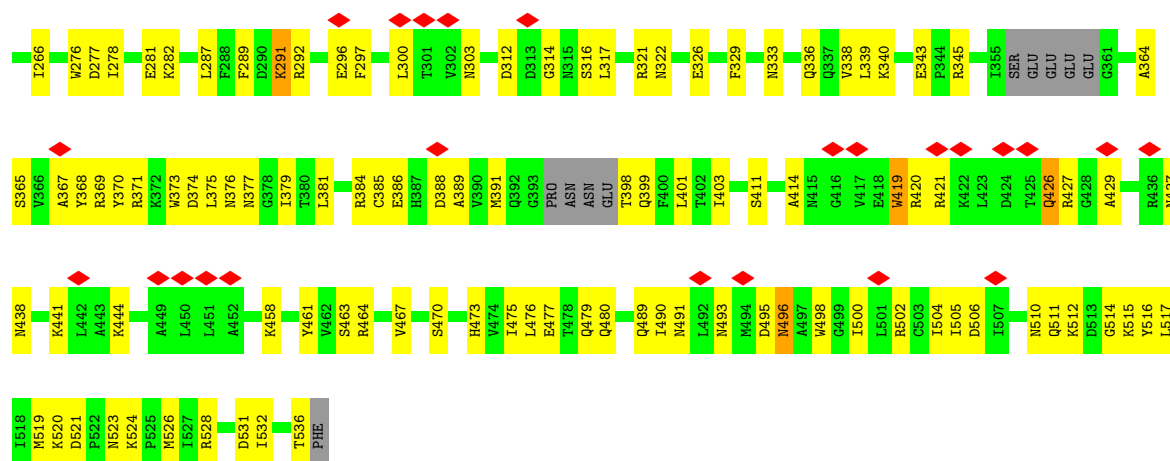


- Molecule 8: Eukaryotic translation initiation factor 3 subunit M



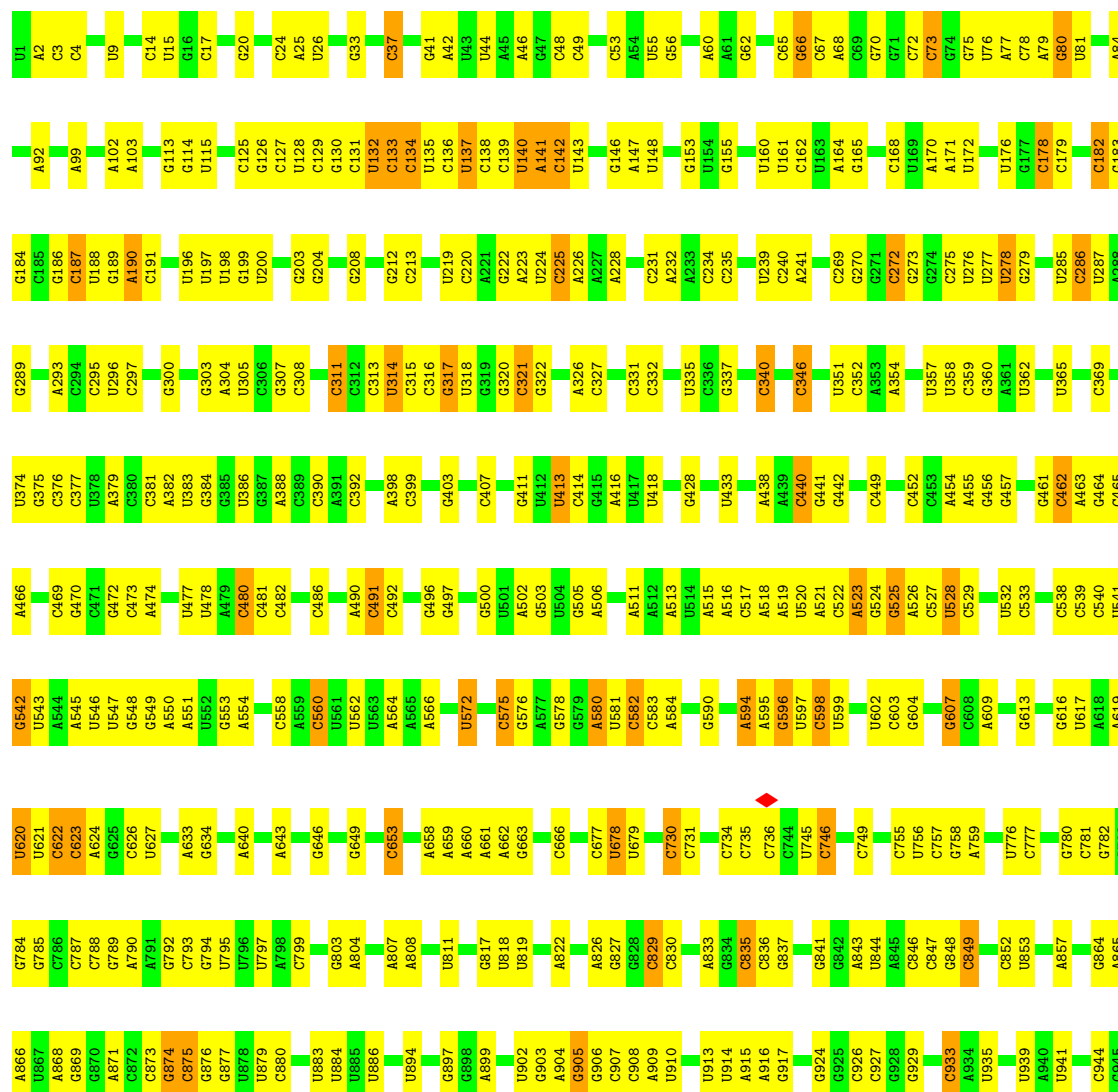
- Molecule 9: EUKARYOTIC TRANSLATION INITIATION FACTOR 3 SUBUNIT D

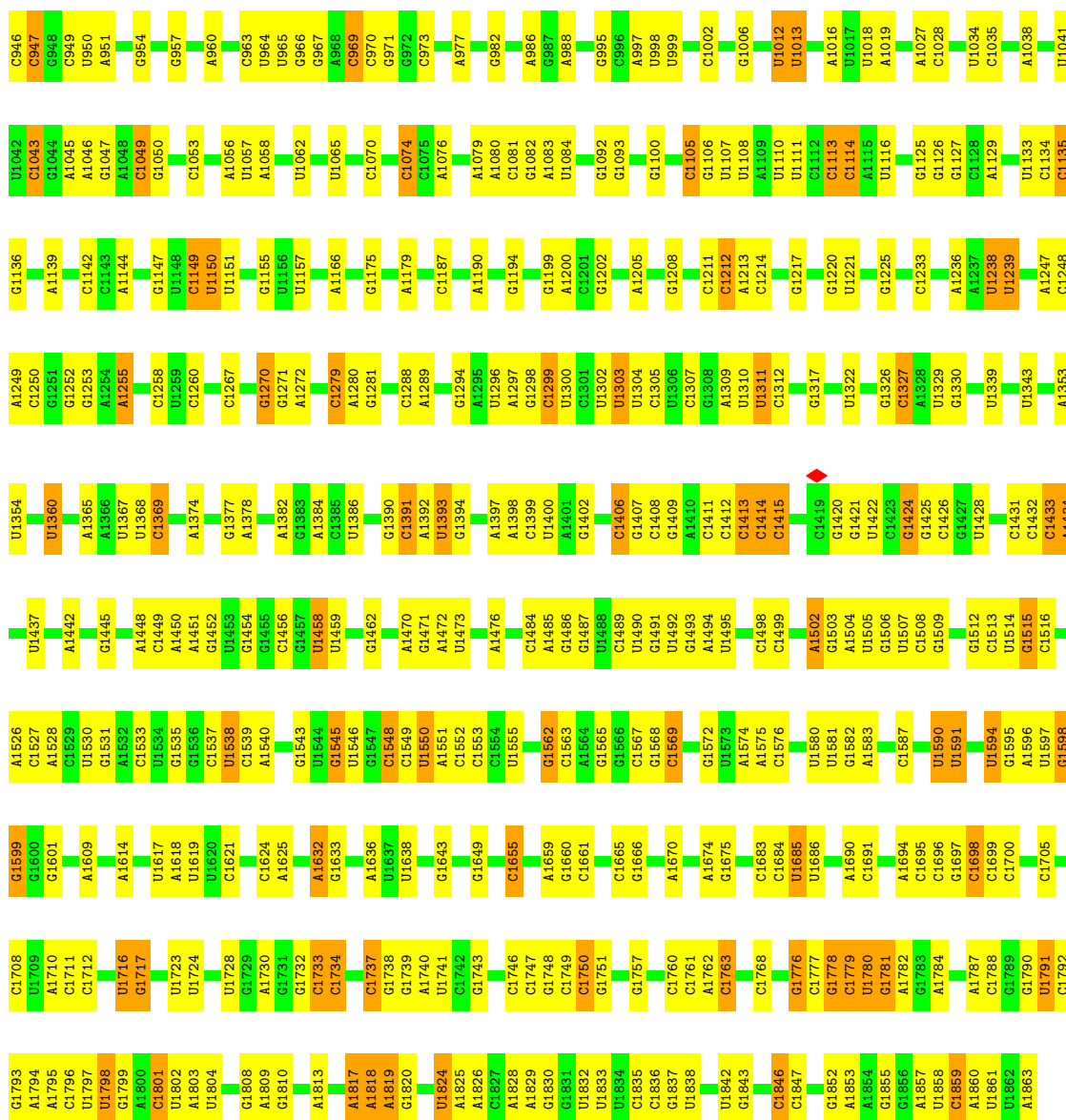




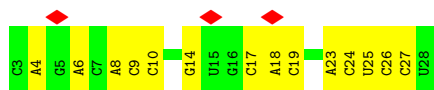
• Molecule 10: 18S ribosomal RNA

Chain A: 54% 39% 7%

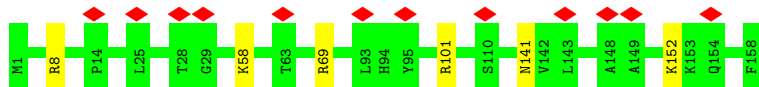




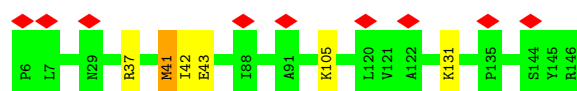
• Molecule 11: Messenger RNA (26-MER)



• Molecule 12: 40S ribosomal protein S11



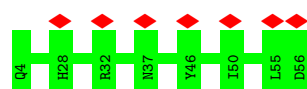
• Molecule 13: 40S ribosomal protein S16



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



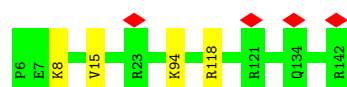
- Molecule 15: 40S ribosomal protein S29



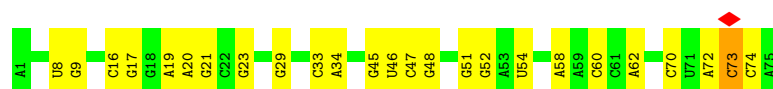
- Molecule 16: 40S ribosomal protein S9



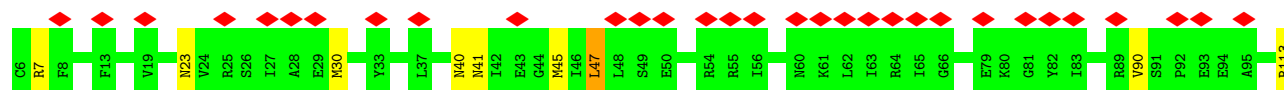
- Molecule 17: 40S ribosomal protein S18

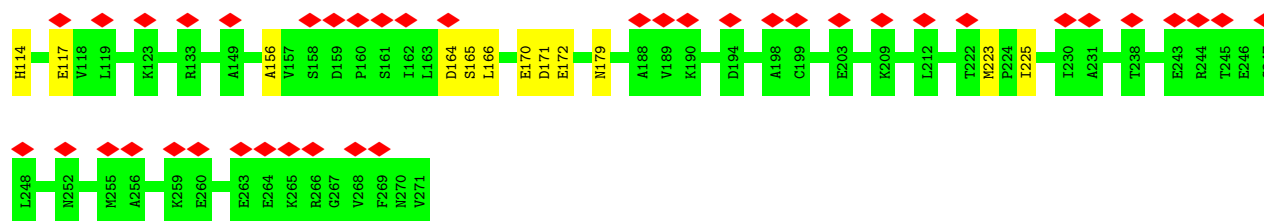


- Molecule 18: Transfer RNA (75-MER)



- Molecule 19: Eukaryotic translation initiation factor 2 subunit 1





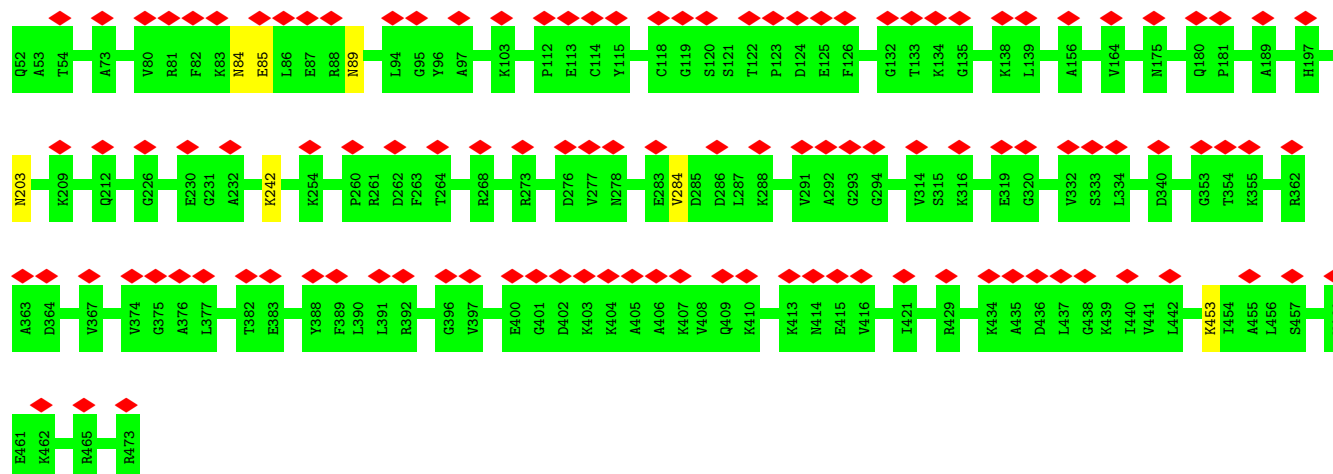
- Molecule 20: 40S ribosomal protein S23



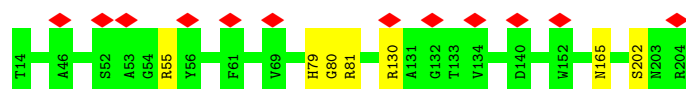
- Molecule 21: 40S ribosomal protein S19



- Molecule 22: Eukaryotic translation initiation factor 2 subunit 3

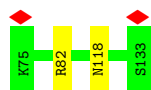


- Molecule 23: 40S ribosomal protein S5



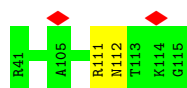
- Molecule 24: 40S ribosomal protein S30

Chain V:  97% .




- Molecule 25: 40S ribosomal protein S25

Chain W:  97% .



- Molecule 26: 40S ribosomal protein S7

Chain X:  93% 6% ..



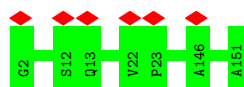
- Molecule 27: 40S ribosomal protein S27

Chain Y:  5% 96% .



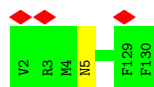
- Molecule 28: 40S ribosomal protein S13

Chain Z:  100% .



- Molecule 29: 40S ribosomal protein S15a

Chain a:  99% .



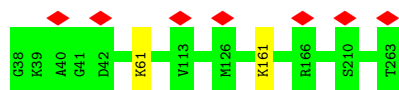
- Molecule 30: 40S ribosomal protein S21

Chain b:  94% 5% .



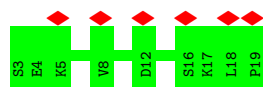
- Molecule 31: 40S ribosomal protein S2

Chain c:  99%



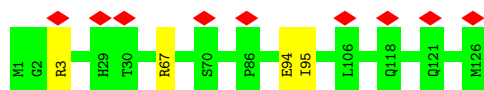
- Molecule 32: EUKARYOTIC TRANSLATION INITIATION FACTOR 2 BETA SUBUNIT (eIF2-Beta)

Chain d:  35% 100%



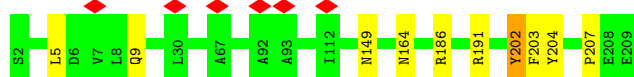
- Molecule 33: 40S ribosomal protein S17

Chain e:  7% 97%



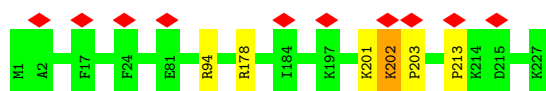
- Molecule 34: 40S ribosomal protein SA

Chain f:  95%



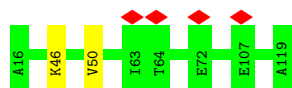
- Molecule 35: 40S ribosomal protein S3

Chain g:  97%



- Molecule 36: 40S ribosomal protein S20

Chain h:  98%

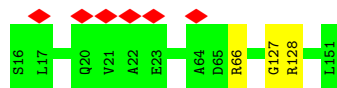


- Molecule 37: 40S ribosomal protein S3a

Chain i:  97%



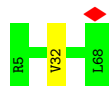
- Molecule 38: 40S ribosomal protein S14



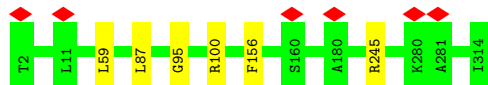
- Molecule 39: 40S ribosomal protein S26



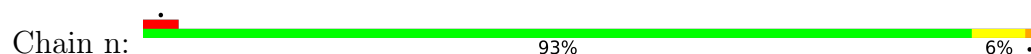
- Molecule 40: 40S ribosomal protein S28



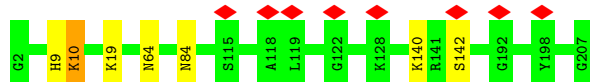
- Molecule 41: Receptor of activated protein C kinase 1



- Molecule 42: 40S ribosomal protein S15



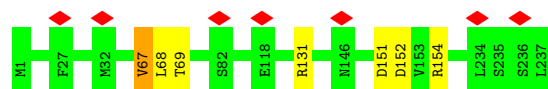
- Molecule 43: 40S ribosomal protein S8



- Molecule 44: Ubiquitin-40S ribosomal protein S27a



- Chain q:  97%



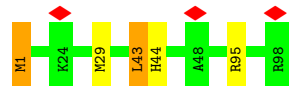
- Chain r:  96%



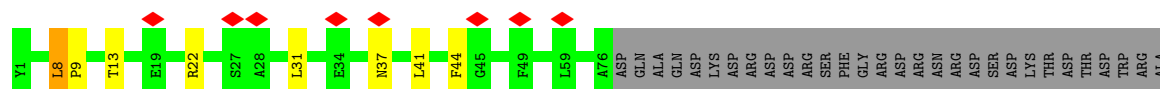
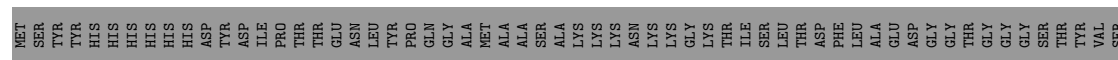
- Chain s:  98%



- Chain t:  95% ..



- Chain u:  11% 88%



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	0.35	0/5021	0.63	1/6781 (0.0%)
2	2	0.34	0/4608	0.57	1/6219 (0.0%)
3	3	0.35	0/3539	0.70	8/4788 (0.2%)
4	4	0.33	0/2149	0.66	0/2920
5	5	0.33	0/2675	0.65	2/3609 (0.1%)
6	6	0.33	0/1773	0.60	0/2398
7	7	0.31	0/3186	0.63	3/4298 (0.1%)
8	8	0.32	0/2964	0.71	5/4000 (0.1%)
9	9	0.29	0/2921	0.54	0/3957
10	A	0.56	1/42353 (0.0%)	1.31	441/66010 (0.7%)
11	F	0.31	0/606	0.95	0/941
12	G	0.36	0/1319	0.65	0/1761
13	H	0.32	0/1142	0.63	0/1528
14	I	0.33	0/2125	0.64	1/2856 (0.0%)
15	J	0.35	0/455	0.58	0/603
16	K	0.32	0/1523	0.60	0/2031
17	L	0.33	0/1158	0.63	0/1548
18	N	0.46	0/1795	1.13	6/2798 (0.2%)
19	P	0.33	0/2178	0.68	0/2935
20	Q	0.32	0/1125	0.60	1/1500 (0.1%)
21	R	0.35	0/1133	0.59	1/1517 (0.1%)
22	S	0.30	0/3267	0.60	1/4415 (0.0%)
23	U	0.31	0/1531	0.56	0/2059
24	V	0.30	0/478	0.69	0/628
25	W	0.36	0/605	0.67	0/810
26	X	0.35	0/1553	0.74	4/2079 (0.2%)
27	Y	0.35	0/673	0.65	1/902 (0.1%)
28	Z	0.31	0/1232	0.54	0/1656
29	a	0.28	0/1051	0.55	0/1406
30	b	0.32	0/627	0.64	0/839
31	c	0.34	0/1779	0.57	0/2399
32	d	0.24	0/149	0.49	0/197
33	e	0.32	0/1032	0.60	0/1383
34	f	0.36	0/1680	0.68	1/2283 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	g	0.32	0/1793	0.60	1/2412 (0.0%)
36	h	0.29	0/832	0.59	0/1117
37	i	0.35	0/1770	0.65	1/2367 (0.0%)
38	j	0.31	0/1029	0.65	0/1380
39	k	0.30	0/803	0.58	0/1076
40	l	0.35	0/509	0.60	0/680
41	m	0.38	0/2494	0.68	1/3394 (0.0%)
42	n	0.36	0/1080	0.68	0/1437
43	o	0.40	0/1709	0.70	1/2278 (0.0%)
44	p	0.44	0/594	0.78	1/786 (0.1%)
45	q	0.35	0/1947	0.64	0/2590
46	r	0.36	0/968	0.66	0/1296
47	s	0.37	0/1083	0.66	1/1437 (0.1%)
48	t	0.34	0/852	0.73	2/1147 (0.2%)
49	u	0.35	0/619	0.83	2/836 (0.2%)
50	w	0.27	0/3407	0.59	1/4620 (0.0%)
All	All	0.43	1/122894 (0.0%)	0.96	488/174907 (0.3%)

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

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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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1311	U	N3-C4	-5.60	1.33	1.38

All (488) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1311	U	N3-C2-O2	-13.33	112.87	122.20
10	A	835	C	N1-C2-O2	11.55	125.83	118.90
10	A	1549	C	N1-C2-O2	11.46	125.77	118.90
10	A	1311	U	N1-C2-O2	11.31	130.72	122.80
10	A	491	C	N1-C2-O2	11.29	125.67	118.90
10	A	539	C	C5-C6-N1	11.21	126.61	121.00
10	A	835	C	C2-N1-C1'	10.99	130.88	118.80
10	A	1327	C	N1-C2-O2	10.67	125.30	118.90
26	X	35	ASP	CB-CG-OD1	10.65	127.88	118.30
10	A	37	C	N1-C2-O2	10.47	125.18	118.90
10	A	440	C	N1-C2-O2	10.46	125.18	118.90
10	A	1549	C	C2-N1-C1'	10.31	130.14	118.80
10	A	1327	C	C2-N1-C1'	10.23	130.06	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	492	C	N1-C2-O2	10.22	125.03	118.90
10	A	835	C	N3-C2-O2	-10.15	114.79	121.90
14	I	13	ALA	C-N-CA	10.13	147.04	121.70
10	A	1311	U	C5-C4-O4	10.06	131.94	125.90
10	A	1513	C	C2-N1-C1'	9.99	129.79	118.80
10	A	829	C	N1-C2-O2	9.91	124.84	118.90
50	w	562	TRP	C-N-CA	9.87	146.38	121.70
10	A	346	C	N1-C2-O2	9.59	124.66	118.90
10	A	849	C	N1-C2-O2	9.47	124.58	118.90
10	A	1422	U	C5-C6-N1	9.45	127.42	122.70
10	A	37	C	N3-C2-O2	-9.36	115.34	121.90
10	A	491	C	N3-C2-O2	-9.19	115.47	121.90
10	A	440	C	C6-N1-C2	-9.15	116.64	120.30
10	A	440	C	N3-C2-O2	-9.15	115.50	121.90
10	A	1549	C	N3-C2-O2	-9.08	115.55	121.90
10	A	1296	U	N3-C2-O2	-9.06	115.86	122.20
10	A	346	C	C2-N1-C1'	9.00	128.69	118.80
10	A	1458	U	N1-C2-O2	8.96	129.07	122.80
10	A	440	C	C2-N1-C1'	8.92	128.61	118.80
10	A	1415	C	N3-C4-N4	8.92	124.24	118.00
10	A	1513	C	N1-C2-O2	8.90	124.24	118.90
10	A	1296	U	N1-C2-O2	8.87	129.01	122.80
10	A	1296	U	C2-N1-C1'	8.83	128.30	117.70
10	A	1012	U	C2-N1-C1'	8.83	128.30	117.70
10	A	1458	U	N3-C2-O2	-8.73	116.09	122.20
10	A	491	C	C2-N1-C1'	8.65	128.31	118.80
10	A	835	C	C6-N1-C2	-8.62	116.85	120.30
10	A	492	C	N3-C2-O2	-8.57	115.90	121.90
10	A	1619	U	C2-N1-C1'	8.52	127.92	117.70
10	A	849	C	C2-N1-C1'	8.51	128.16	118.80
10	A	914	U	N1-C2-O2	8.40	128.68	122.80
10	A	1546	U	N1-C2-O2	8.35	128.64	122.80
10	A	1113	C	N1-C2-O2	8.32	123.89	118.90
10	A	178	C	N1-C2-O2	8.28	123.87	118.90
10	A	1414	C	N1-C2-O2	8.19	123.82	118.90
10	A	849	C	N3-C2-O2	-8.16	116.19	121.90
10	A	491	C	C6-N1-C2	-8.14	117.04	120.30
10	A	1327	C	N3-C2-O2	-8.08	116.24	121.90
10	A	1859	C	N1-C2-O2	8.07	123.74	118.90
10	A	598	C	N1-C2-O2	7.90	123.64	118.90
10	A	1360	U	C2-N1-C1'	7.89	127.17	117.70
10	A	1546	U	C2-N1-C1'	7.89	127.17	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1360	U	N1-C2-O2	7.84	128.29	122.80
10	A	1513	C	C6-N1-C1'	-7.84	111.39	120.80
10	A	1012	U	N3-C2-O2	-7.80	116.74	122.20
10	A	1414	C	C2-N1-C1'	7.79	127.37	118.80
10	A	492	C	C2-N1-C1'	7.76	127.33	118.80
10	A	1311	U	N3-C4-O4	-7.70	114.01	119.40
10	A	381	C	C6-N1-C2	-7.69	117.22	120.30
10	A	1619	U	N1-C2-O2	7.63	128.14	122.80
5	5	222	SER	N-CA-C	7.58	131.47	111.00
10	A	970	C	C6-N1-C2	-7.56	117.28	120.30
10	A	346	C	N3-C2-O2	-7.51	116.64	121.90
10	A	1621	C	N3-C2-O2	-7.47	116.67	121.90
3	3	268	ARG	C-N-CA	7.46	140.36	121.70
10	A	187	C	N1-C2-O2	7.45	123.37	118.90
10	A	829	C	N3-C2-O2	-7.42	116.70	121.90
10	A	1413	C	C6-N1-C2	-7.42	117.33	120.30
10	A	1053	C	C2-N1-C1'	7.42	126.97	118.80
10	A	1621	C	N1-C2-O2	7.40	123.34	118.90
10	A	1012	U	N1-C2-O2	7.37	127.96	122.80
10	A	1135	C	C2-N1-C1'	7.32	126.85	118.80
10	A	1327	C	C6-N1-C1'	-7.32	112.02	120.80
10	A	1310	U	O4'-C1'-N1	7.30	114.04	108.20
10	A	1619	U	N3-C2-O2	-7.30	117.09	122.20
10	A	1018	U	C2-N1-C1'	7.29	126.45	117.70
10	A	1074	C	N1-C2-O2	7.28	123.27	118.90
10	A	1794	A	N7-C8-N9	7.28	117.44	113.80
10	A	1546	U	N3-C2-O2	-7.27	117.11	122.20
10	A	730	C	N1-C2-O2	7.25	123.25	118.90
10	A	620	U	C2-N1-C1'	7.24	126.39	117.70
10	A	1384	A	N1-C6-N6	7.23	122.94	118.60
10	A	1549	C	C6-N1-C1'	-7.22	112.13	120.80
10	A	469	C	C5-C6-N1	7.22	124.61	121.00
10	A	1515	G	C4-N9-C1'	7.22	135.89	126.50
10	A	1214	C	C5-C6-N1	7.21	124.61	121.00
10	A	1737	C	N1-C2-O2	7.19	123.22	118.90
10	A	225	C	N1-C2-O2	7.19	123.21	118.90
10	A	1655	C	N1-C2-O2	7.18	123.21	118.90
10	A	835	C	C6-N1-C1'	-7.16	112.21	120.80
10	A	914	U	N3-C2-O2	-7.14	117.20	122.20
8	8	115	LYS	C-N-CA	7.14	139.55	121.70
10	A	1458	U	C2-N1-C1'	7.13	126.26	117.70
10	A	525	G	C6-C5-N7	-7.12	126.13	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	7	348	SER	C-N-CA	7.11	139.48	121.70
10	A	141	A	P-O3'-C3'	7.11	128.23	119.70
3	3	38	LEU	CB-CG-CD1	7.11	123.08	111.00
10	A	37	C	C2-N1-C1'	7.10	126.61	118.80
10	A	1105	C	C2-N1-C1'	7.09	126.60	118.80
37	i	48	LEU	CA-CB-CG	7.07	131.56	115.30
41	m	87	LEU	CA-CB-CG	7.07	131.55	115.30
10	A	880	C	C6-N1-C2	-7.05	117.48	120.30
10	A	622	C	C6-N1-C2	-7.05	117.48	120.30
10	A	346	C	C6-N1-C1'	-7.03	112.36	120.80
10	A	178	C	C2-N1-C1'	7.03	126.53	118.80
10	A	317	G	P-O3'-C3'	6.99	128.08	119.70
10	A	914	U	C2-N1-C1'	6.98	126.08	117.70
10	A	1018	U	N1-C2-O2	6.98	127.69	122.80
10	A	1779	C	O4'-C1'-N1	6.96	113.76	108.20
10	A	539	C	C6-N1-C2	-6.95	117.52	120.30
10	A	1113	C	C2-N1-C1'	6.93	126.42	118.80
10	A	927	C	N1-C2-O2	6.92	123.05	118.90
10	A	37	C	C6-N1-C2	-6.92	117.53	120.30
10	A	1105	C	N1-C2-O2	6.92	123.05	118.90
10	A	1415	C	C5-C4-N4	-6.92	115.36	120.20
10	A	730	C	C5-C6-N1	6.90	124.45	121.00
10	A	469	C	C6-N1-C2	-6.89	117.55	120.30
10	A	491	C	C5-C6-N1	6.87	124.43	121.00
10	A	1515	G	N3-C4-C5	-6.84	125.18	128.60
10	A	525	G	N9-C4-C5	-6.83	102.67	105.40
18	N	60	C	C5-C6-N1	6.82	124.41	121.00
10	A	1449	C	N3-C2-O2	-6.81	117.14	121.90
10	A	849	C	C6-N1-C2	-6.80	117.58	120.30
10	A	1449	C	C2-N1-C1'	6.80	126.28	118.80
10	A	1859	C	C2-N1-C1'	6.79	126.27	118.80
10	A	1621	C	C6-N1-C2	-6.77	117.59	120.30
10	A	1698	C	N1-C2-O2	6.77	122.96	118.90
10	A	14	C	C6-N1-C2	-6.75	117.60	120.30
10	A	1716	U	C2-N1-C1'	6.75	125.79	117.70
10	A	649	G	C4-N9-C1'	6.73	135.25	126.50
10	A	1414	C	N3-C2-O2	-6.73	117.19	121.90
10	A	1187	C	C6-N1-C2	-6.73	117.61	120.30
10	A	998	U	N1-C2-O2	6.73	127.51	122.80
3	3	38	LEU	CB-CG-CD2	-6.71	99.58	111.00
10	A	880	C	C5-C6-N1	6.69	124.35	121.00
10	A	620	U	N1-C2-O2	6.68	127.48	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1299	C	C2-N1-C1'	6.68	126.14	118.80
10	A	1449	C	N1-C2-O2	6.67	122.90	118.90
10	A	596	G	C4-N9-C1'	6.66	135.16	126.50
10	A	1548	C	C2-N1-C1'	6.66	126.12	118.80
10	A	327	C	C6-N1-C2	-6.66	117.64	120.30
10	A	1384	A	C5-C6-N6	-6.66	118.37	123.70
10	A	66	G	OP1-P-O3'	6.62	119.75	105.20
10	A	178	C	N3-C2-O2	-6.62	117.27	121.90
10	A	480	C	C5-C6-N1	6.60	124.30	121.00
10	A	649	G	C6-C5-N7	-6.58	126.45	130.40
10	A	539	C	C4-C5-C6	-6.58	114.11	117.40
10	A	1548	C	N1-C2-O2	6.56	122.84	118.90
10	A	528	U	C5-C6-N1	6.55	125.97	122.70
10	A	1563	C	N1-C2-O2	6.52	122.81	118.90
10	A	998	U	N3-C2-O2	-6.52	117.64	122.20
10	A	622	C	C5-C6-N1	6.50	124.25	121.00
3	3	38	LEU	CA-CB-CG	6.49	130.23	115.30
10	A	178	C	C6-N1-C2	-6.48	117.71	120.30
10	A	1549	C	C6-N1-C2	-6.48	117.71	120.30
10	A	1859	C	N3-C2-O2	-6.47	117.37	121.90
10	A	1433	C	N1-C2-O2	6.47	122.78	118.90
43	o	142	SER	C-N-CA	6.47	137.87	121.70
10	A	1214	C	C6-N1-C2	-6.43	117.73	120.30
10	A	649	G	N3-C4-N9	6.42	129.85	126.00
10	A	1515	G	N3-C4-N9	6.42	129.85	126.00
10	A	15	U	C5-C6-N1	6.41	125.90	122.70
10	A	1836	C	N1-C2-O2	6.40	122.74	118.90
10	A	1411	C	C6-N1-C2	-6.39	117.74	120.30
10	A	1299	C	C6-N1-C1'	-6.39	113.14	120.80
10	A	1053	C	N1-C2-O2	6.37	122.72	118.90
10	A	1415	C	C4-C5-C6	6.37	120.58	117.40
10	A	525	G	C4-C5-N7	6.36	113.34	110.80
10	A	480	C	C6-N1-C2	-6.35	117.76	120.30
10	A	819	U	C2-N1-C1'	6.35	125.31	117.70
10	A	1473	U	C2-N1-C1'	6.34	125.31	117.70
10	A	1053	C	C6-N1-C1'	-6.34	113.19	120.80
10	A	1360	U	N3-C2-O2	-6.33	117.77	122.20
10	A	308	C	N3-C2-O2	-6.32	117.48	121.90
10	A	1212	C	C2-N1-C1'	6.32	125.75	118.80
10	A	440	C	C5-C6-N1	6.31	124.16	121.00
10	A	835	C	C5-C6-N1	6.28	124.14	121.00
10	A	1105	C	N3-C2-O2	-6.27	117.51	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1310	U	C2-N1-C1'	6.26	125.22	117.70
10	A	1513	C	N3-C2-O2	-6.24	117.53	121.90
26	X	17	ASP	N-CA-C	6.23	127.83	111.00
10	A	678	U	C2-N1-C1'	6.23	125.18	117.70
10	A	1794	A	C4-N9-C1'	6.23	137.51	126.30
10	A	607	G	N9-C4-C5	-6.22	102.91	105.40
10	A	730	C	C2-N1-C1'	6.22	125.64	118.80
10	A	178	C	C5-C6-N1	6.21	124.11	121.00
10	A	597	U	C2-N1-C1'	6.20	125.14	117.70
18	N	70	C	C6-N1-C2	-6.20	117.82	120.30
10	A	287	U	N1-C2-O2	6.20	127.14	122.80
10	A	1114	C	C2-N1-C1'	6.19	125.61	118.80
10	A	649	G	C8-N9-C1'	-6.19	118.96	127.00
10	A	492	C	C6-N1-C2	-6.18	117.83	120.30
10	A	462	C	N1-C2-O2	6.18	122.61	118.90
10	A	308	C	N1-C2-O2	6.17	122.60	118.90
10	A	598	C	C2-N1-C1'	6.16	125.58	118.80
10	A	933	C	C6-N1-C2	-6.16	117.83	120.30
18	N	73	C	P-O3'-C3'	6.16	127.09	119.70
10	A	1776	G	C8-N9-C4	-6.15	103.94	106.40
10	A	730	C	C6-N1-C2	-6.13	117.85	120.30
10	A	1377	G	N3-C2-N2	-6.12	115.62	119.90
3	3	143	ASN	C-N-CA	6.12	136.99	121.70
10	A	413	U	N1-C2-O2	6.11	127.08	122.80
10	A	1591	U	C5-C6-N1	6.11	125.75	122.70
10	A	311	C	N1-C2-O2	6.10	122.56	118.90
48	t	43	LEU	CA-CB-CG	6.09	129.30	115.30
10	A	1149	C	N1-C2-O2	6.07	122.54	118.90
10	A	1150	U	C2-N1-C1'	6.07	124.99	117.70
8	8	226	LEU	CA-CB-CG	6.07	129.26	115.30
10	A	596	G	N3-C4-N9	6.04	129.63	126.00
10	A	1619	U	C6-N1-C1'	-6.02	112.77	121.20
10	A	572	U	N3-C2-O2	-6.02	117.99	122.20
10	A	572	U	C2-N1-C1'	6.01	124.92	117.70
10	A	1716	U	N1-C2-O2	6.00	127.00	122.80
10	A	1791	U	C5-C6-N1	6.00	125.70	122.70
49	u	8	LEU	CA-CB-CG	6.00	129.09	115.30
10	A	190	A	OP1-P-O3'	5.99	118.37	105.20
10	A	1685	U	N1-C2-O2	5.98	126.99	122.80
10	A	1780	U	C5-C6-N1	5.98	125.69	122.70
10	A	1473	U	N1-C2-O2	5.98	126.98	122.80
10	A	407	C	N1-C2-O2	5.97	122.48	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1846	C	C6-N1-C2	-5.96	117.91	120.30
10	A	162	C	N1-C2-O2	5.96	122.48	118.90
10	A	598	C	C5-C6-N1	5.96	123.98	121.00
10	A	1113	C	N3-C2-O2	-5.95	117.73	121.90
10	A	14	C	N3-C2-O2	-5.95	117.73	121.90
10	A	1043	C	C6-N1-C2	-5.95	117.92	120.30
10	A	1327	C	C6-N1-C2	-5.94	117.92	120.30
3	3	257	LEU	CA-CB-CG	5.93	128.94	115.30
10	A	1212	C	N1-C2-O2	5.91	122.44	118.90
10	A	1563	C	N3-C2-O2	-5.90	117.77	121.90
10	A	1434	A	N1-C6-N6	5.90	122.14	118.60
10	A	321	C	O4'-C1'-N1	5.89	112.91	108.20
10	A	927	C	C6-N1-C2	-5.89	117.94	120.30
10	A	1716	U	N3-C2-O2	-5.88	118.08	122.20
10	A	369	C	C5-C6-N1	5.88	123.94	121.00
10	A	1599	G	N3-C4-N9	5.87	129.52	126.00
10	A	1546	U	C6-N1-C1'	-5.86	113.00	121.20
10	A	542	G	P-O3'-C3'	5.86	126.73	119.70
10	A	525	G	N3-C4-N9	5.85	129.51	126.00
10	A	384	G	C4-N9-C1'	5.85	134.10	126.50
10	A	1533	C	N1-C2-O2	5.84	122.41	118.90
10	A	133	C	P-O3'-C3'	5.84	126.70	119.70
10	A	927	C	C5-C6-N1	5.83	123.91	121.00
10	A	787	C	C6-N1-C2	-5.82	117.97	120.30
10	A	799	C	C6-N1-C2	-5.82	117.97	120.30
10	A	1655	C	C2-N1-C1'	5.82	125.20	118.80
10	A	1018	U	N3-C2-O2	-5.82	118.13	122.20
10	A	1299	C	O4'-C1'-N1	5.82	112.85	108.20
10	A	286	C	N1-C2-O2	5.81	122.39	118.90
10	A	1794	A	C5-N7-C8	-5.78	101.01	103.90
10	A	944	C	C6-N1-C2	-5.78	117.99	120.30
10	A	1414	C	C6-N1-C1'	-5.78	113.87	120.80
49	u	41	LEU	CA-CB-CG	5.76	128.56	115.30
8	8	279	LEU	CA-CB-CG	5.76	128.54	115.30
10	A	572	U	N1-C2-O2	5.76	126.83	122.80
10	A	1013	U	N1-C2-O2	5.76	126.83	122.80
10	A	596	G	N3-C4-C5	-5.75	125.72	128.60
10	A	1530	U	C2-N1-C1'	5.74	124.59	117.70
3	3	189	LEU	CA-CB-CG	5.74	128.50	115.30
10	A	1384	A	C4-C5-N7	5.74	113.57	110.70
10	A	1515	G	C8-N9-C1'	-5.74	119.54	127.00
10	A	80	G	C4-N9-C1'	5.73	133.95	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	582	C	N1-C2-O2	5.73	122.34	118.90
10	A	1708	C	N1-C2-O2	5.72	122.33	118.90
10	A	1632	A	P-O3'-C3'	5.72	126.56	119.70
10	A	626	C	N1-C2-O2	5.71	122.33	118.90
10	A	1279	C	C5-C6-N1	5.71	123.86	121.00
10	A	947	C	C6-N1-C2	-5.71	118.02	120.30
10	A	165	G	C4-N9-C1'	5.70	133.91	126.50
10	A	1456	C	C6-N1-C2	-5.69	118.02	120.30
10	A	132	U	C2-N1-C1'	5.69	124.53	117.70
10	A	465	C	C5-C6-N1	5.69	123.84	121.00
10	A	1711	C	C6-N1-C2	-5.69	118.02	120.30
10	A	1599	G	N3-C4-C5	-5.68	125.76	128.60
1	1	22	GLY	N-CA-C	-5.68	98.90	113.10
10	A	392	C	C5-C6-N1	5.68	123.84	121.00
18	N	52	G	C5-C6-O6	-5.68	125.19	128.60
10	A	1768	C	C5-C6-N1	5.67	123.83	121.00
48	t	1	MET	C-N-CA	5.67	135.87	121.70
10	A	1763	C	C6-N1-C2	-5.66	118.04	120.30
10	A	142	C	C2-N1-C1'	5.65	125.01	118.80
10	A	1776	G	N7-C8-N9	5.64	115.92	113.10
10	A	1424	G	C8-N9-C1'	5.64	134.33	127.00
10	A	1594	U	C2-N1-C1'	5.63	124.46	117.70
10	A	134	C	C6-N1-C2	-5.63	118.05	120.30
10	A	677	C	N1-C2-O2	5.63	122.28	118.90
10	A	1528	A	N1-C6-N6	-5.62	115.23	118.60
10	A	1303	U	C5-C6-N1	5.62	125.51	122.70
10	A	1835	C	N1-C2-O2	5.62	122.27	118.90
10	A	320	G	N3-C4-N9	5.62	129.37	126.00
10	A	1092	G	C4-N9-C1'	-5.61	119.20	126.50
10	A	1449	C	C6-N1-C2	-5.61	118.06	120.30
10	A	14	C	N1-C2-O2	5.61	122.27	118.90
34	f	5	LEU	CA-CB-CG	5.61	128.20	115.30
10	A	1750	C	P-O3'-C3'	5.61	126.43	119.70
10	A	414	C	N1-C2-O2	5.60	122.26	118.90
10	A	954	G	C4-N9-C1'	5.59	133.77	126.50
10	A	523	A	O4'-C1'-N9	5.59	112.67	108.20
10	A	1074	C	N3-C2-O2	-5.59	117.99	121.90
10	A	1550	U	N1-C2-O2	5.58	126.71	122.80
10	A	1580	U	N3-C2-O2	-5.58	118.30	122.20
2	2	391	THR	C-N-CA	5.57	135.63	121.70
10	A	620	U	N3-C2-O2	-5.57	118.30	122.20
10	A	165	G	C8-N9-C1'	-5.57	119.76	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	340	C	C6-N1-C2	-5.56	118.08	120.30
10	A	73	C	N1-C2-O2	5.56	122.23	118.90
10	A	1798	U	C5-C6-N1	5.56	125.48	122.70
10	A	1723	U	N1-C2-O2	5.55	126.69	122.80
10	A	1733	C	N1-C2-O2	5.55	122.23	118.90
10	A	596	G	C8-N9-C1'	-5.54	119.79	127.00
10	A	1296	U	C5-C6-N1	5.54	125.47	122.70
10	A	1413	C	C5-C6-N1	5.54	123.77	121.00
10	A	1824	U	P-O3'-C3'	5.54	126.34	119.70
10	A	529	C	C5-C6-N1	5.53	123.77	121.00
10	A	66	G	O5'-P-OP1	-5.52	100.73	105.70
22	S	84	ASN	C-N-CA	5.52	135.51	121.70
10	A	1562	G	C4-N9-C1'	5.52	133.68	126.50
10	A	392	C	C6-N1-C2	-5.52	118.09	120.30
10	A	1296	U	C6-N1-C2	-5.52	117.69	121.00
10	A	575	C	C5-C6-N1	5.52	123.76	121.00
10	A	1549	C	C5-C6-N1	5.50	123.75	121.00
10	A	225	C	N3-C4-C5	5.49	124.10	121.90
10	A	849	C	C6-N1-C1'	-5.49	114.21	120.80
10	A	1260	C	C6-N1-C2	5.48	122.49	120.30
10	A	1238	U	N1-C2-O2	5.48	126.63	122.80
26	X	69	LEU	CA-CB-CG	5.48	127.90	115.30
10	A	597	U	N1-C2-O2	5.47	126.63	122.80
10	A	1545	G	O4'-C1'-N9	5.46	112.57	108.20
10	A	1794	A	C8-N9-C1'	-5.45	117.88	127.70
10	A	132	U	N1-C2-O2	5.45	126.61	122.80
27	Y	63	LEU	CA-CB-CG	5.45	127.83	115.30
3	3	50	MET	C-N-CA	5.43	135.27	121.70
10	A	137	U	C2-N1-C1'	5.42	124.21	117.70
10	A	1233	C	N1-C2-O2	5.42	122.15	118.90
10	A	1842	U	C5-C6-N1	5.42	125.41	122.70
10	A	1049	C	C6-N1-C2	-5.41	118.14	120.30
10	A	413	U	N3-C2-O2	-5.41	118.41	122.20
10	A	819	U	N3-C2-O2	-5.40	118.42	122.20
10	A	1255	A	C2-N3-C4	5.40	113.30	110.60
10	A	1594	U	P-O3'-C3'	5.40	126.18	119.70
10	A	1135	C	N1-C2-O2	5.40	122.14	118.90
10	A	1836	C	C6-N1-C2	-5.40	118.14	120.30
10	A	1360	U	C6-N1-C1'	-5.39	113.65	121.20
10	A	1492	U	C5-C6-N1	5.39	125.40	122.70
10	A	623	C	C6-N1-C2	-5.39	118.14	120.30
10	A	213	C	N1-C2-O2	5.39	122.13	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	533	C	C6-N1-C2	-5.39	118.14	120.30
10	A	594	A	P-O3'-C3'	5.38	126.16	119.70
10	A	452	C	C6-N1-C2	-5.38	118.15	120.30
10	A	517	C	C6-N1-C2	-5.37	118.15	120.30
10	A	1661	C	N1-C2-O2	5.37	122.12	118.90
10	A	1424	G	C4-N9-C1'	-5.36	119.53	126.50
10	A	905	G	C8-N9-C1'	5.36	133.97	127.00
10	A	142	C	N1-C2-O2	5.36	122.11	118.90
10	A	272	C	C6-N1-C2	-5.35	118.16	120.30
10	A	1502	A	N7-C8-N9	5.35	116.48	113.80
10	A	1802	U	C6-N1-C2	-5.35	117.79	121.00
10	A	377	C	C6-N1-C2	-5.35	118.16	120.30
10	A	1327	C	C5-C6-N1	5.35	123.67	121.00
10	A	1598	G	N1-C6-O6	5.35	123.11	119.90
10	A	1012	U	C6-N1-C1'	-5.35	113.71	121.20
10	A	597	U	N3-C2-O2	-5.33	118.47	122.20
10	A	1239	U	N1-C2-O2	5.33	126.53	122.80
10	A	1655	C	N3-C2-O2	-5.33	118.17	121.90
10	A	231	C	C6-N1-C2	-5.33	118.17	120.30
10	A	1187	C	C5-C6-N1	5.33	123.66	121.00
10	A	1685	U	N3-C2-O2	-5.32	118.47	122.20
10	A	1135	C	C6-N1-C1'	-5.32	114.42	120.80
10	A	529	C	C6-N1-C2	-5.32	118.17	120.30
10	A	746	C	C6-N1-C2	-5.32	118.17	120.30
10	A	1819	A	C2-N3-C4	5.31	113.26	110.60
10	A	1074	C	C2-N1-C1'	5.31	124.64	118.80
10	A	1108	U	N1-C2-O2	5.30	126.51	122.80
10	A	1384	A	C5-N7-C8	-5.30	101.25	103.90
20	Q	17	ARG	NE-CZ-NH2	-5.30	117.65	120.30
10	A	819	U	N1-C2-O2	5.29	126.50	122.80
10	A	1270	G	N3-C4-N9	5.29	129.17	126.00
10	A	1013	U	N3-C2-O2	-5.29	118.50	122.20
10	A	386	U	C2-N1-C1'	-5.28	111.37	117.70
10	A	1310	U	C5-C6-N1	5.28	125.34	122.70
10	A	935	U	N1-C2-O2	5.27	126.49	122.80
10	A	1012	U	C5-C6-N1	5.25	125.33	122.70
10	A	905	G	N3-C4-N9	-5.25	122.85	126.00
10	A	1538	U	P-O3'-C3'	5.25	126.00	119.70
10	A	627	U	C6-N1-C2	-5.25	117.85	121.00
10	A	1043	C	N3-C2-O2	-5.25	118.22	121.90
10	A	1473	U	N3-C2-O2	-5.25	118.53	122.20
10	A	1311	U	C6-N1-C2	-5.24	117.85	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1828	A	N1-C6-N6	-5.24	115.46	118.60
10	A	1150	U	N1-C2-O2	5.24	126.47	122.80
10	A	1717	G	C4-C5-N7	5.24	112.89	110.80
10	A	580	A	C2-N3-C4	5.23	113.22	110.60
10	A	1778	G	N9-C4-C5	-5.23	103.31	105.40
10	A	225	C	N3-C2-O2	-5.23	118.24	121.90
10	A	560	C	N1-C2-O2	5.22	122.03	118.90
10	A	1053	C	O4'-C1'-N1	5.22	112.38	108.20
10	A	626	C	C5-C6-N1	5.22	123.61	121.00
8	8	219	LEU	CB-CG-CD2	-5.22	102.13	111.00
10	A	140	U	P-O3'-C3'	5.22	125.96	119.70
10	A	48	C	C6-N1-C2	-5.21	118.22	120.30
10	A	1508	C	C6-N1-C2	-5.21	118.22	120.30
10	A	80	G	N7-C8-N9	5.21	115.70	113.10
10	A	1780	U	C6-N1-C2	-5.21	117.88	121.00
10	A	287	U	N3-C2-O2	-5.20	118.56	122.20
10	A	1092	G	N3-C4-C5	5.20	131.20	128.60
10	A	1393	U	N1-C2-O2	5.20	126.44	122.80
10	A	1734	C	C5-C6-N1	5.20	123.60	121.00
10	A	1781	G	N7-C8-N9	5.20	115.70	113.10
10	A	140	U	OP1-P-O3'	5.19	116.62	105.20
10	A	1512	G	C5-C6-O6	-5.18	125.49	128.60
10	A	1590	U	C5-C6-N1	5.18	125.29	122.70
10	A	960	A	C5-C6-N1	5.18	120.29	117.70
10	A	1801	C	C6-N1-C2	-5.17	118.23	120.30
47	s	86	GLU	N-CA-C	5.17	124.96	111.00
10	A	491	C	C6-N1-C1'	-5.16	114.61	120.80
10	A	539	C	C2-N1-C1'	5.15	124.47	118.80
10	A	874	G	C5-C6-O6	-5.15	125.51	128.60
10	A	1267	C	N1-C2-O2	5.15	121.99	118.90
21	R	28	LEU	CA-CB-CG	5.15	127.15	115.30
10	A	80	G	C8-N9-C1'	-5.15	120.31	127.00
10	A	1818	A	C2-N3-C4	5.15	113.17	110.60
10	A	1413	C	C6-N1-C1'	5.15	126.98	120.80
10	A	1550	U	C2-N1-C1'	5.14	123.87	117.70
10	A	1369	C	C5-C6-N1	5.14	123.57	121.00
10	A	1296	U	C6-N1-C1'	-5.14	114.01	121.20
10	A	730	C	N3-C2-O2	-5.13	118.31	121.90
8	8	334	VAL	C-N-CA	5.13	134.52	121.70
10	A	1221	U	C5-C6-N1	5.13	125.27	122.70
10	A	1562	G	C8-N9-C1'	-5.13	120.33	127.00
10	A	1621	C	C2-N1-C1'	5.13	124.44	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	p	146	LEU	CA-CB-CG	5.13	127.10	115.30
10	A	452	C	C5-C6-N1	5.12	123.56	121.00
10	A	1399	C	N1-C2-O2	5.12	121.97	118.90
10	A	70	G	C5-C6-O6	-5.11	125.53	128.60
10	A	927	C	N3-C2-O2	-5.11	118.33	121.90
10	A	314	U	C2-N1-C1'	5.11	123.83	117.70
10	A	946	C	C6-N1-C2	-5.11	118.26	120.30
35	g	201	LYS	C-N-CA	5.11	134.46	121.70
5	5	50	ILE	CG1-CB-CG2	-5.10	100.17	111.40
10	A	620	U	C6-N1-C1'	-5.10	114.06	121.20
10	A	1550	U	N3-C2-O2	-5.10	118.63	122.20
10	A	137	U	N1-C2-O2	5.10	126.37	122.80
10	A	225	C	P-O3'-C3'	5.10	125.81	119.70
10	A	1836	C	N3-C2-O2	-5.10	118.33	121.90
10	A	1105	C	C6-N1-C2	-5.09	118.26	120.30
10	A	1632	A	OP2-P-O3'	5.09	116.39	105.20
10	A	1599	G	C4-N9-C1'	5.08	133.11	126.50
7	7	486	PHE	C-N-CA	5.08	134.41	121.70
10	A	449	C	N1-C2-O2	5.08	121.95	118.90
10	A	1166	A	C4-C5-C6	-5.07	114.46	117.00
10	A	187	C	C2-N1-C1'	5.07	124.38	118.80
10	A	1384	A	N9-C4-C5	-5.07	103.77	105.80
10	A	787	C	C5-C6-N1	5.07	123.53	121.00
10	A	1114	C	N1-C2-O2	5.07	121.94	118.90
26	X	122	LEU	CA-CB-CG	5.07	126.96	115.30
10	A	384	G	C8-N9-C1'	-5.07	120.41	127.00
10	A	1406	C	N1-C2-O2	5.07	121.94	118.90
10	A	1847	C	N1-C2-O2	5.06	121.94	118.90
10	A	607	G	C4-C5-N7	5.06	112.83	110.80
10	A	1391	C	P-O3'-C3'	5.06	125.78	119.70
10	A	1796	C	C6-N1-C2	-5.06	118.28	120.30
18	N	70	C	N3-C2-O2	-5.06	118.36	121.90
10	A	440	C	C6-N1-C1'	-5.06	114.73	120.80
7	7	379	PRO	C-N-CA	5.05	134.34	121.70
10	A	1012	U	C6-N1-C2	-5.05	117.97	121.00
10	A	1303	U	N1-C2-O2	5.05	126.33	122.80
10	A	1515	G	C2-N3-C4	5.04	114.42	111.90
10	A	666	C	C6-N1-C2	-5.03	118.29	120.30
10	A	1233	C	N3-C2-O2	-5.03	118.38	121.90
10	A	182	C	N1-C2-O2	5.03	121.92	118.90
10	A	66	G	P-O3'-C3'	5.03	125.73	119.70
10	A	969	C	C6-N1-C2	-5.02	118.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	492	C	C6-N1-C1'	-5.02	114.77	120.80
18	N	52	G	N1-C6-O6	5.02	122.91	119.90
10	A	278	U	P-O3'-C3'	5.02	125.72	119.70
10	A	875	C	N1-C2-O2	5.01	121.91	118.90
10	A	133	C	OP1-P-O3'	5.01	116.23	105.20
10	A	1569	C	N1-C2-O2	5.01	121.91	118.90
10	A	1817	A	P-O3'-C3'	5.01	125.71	119.70
10	A	653	C	C5-C6-N1	5.01	123.50	121.00
10	A	1107	U	N1-C2-O2	5.01	126.31	122.80
10	A	1705	C	N1-C2-O2	5.01	121.91	118.90
10	A	1018	U	C6-N1-C1'	-5.01	114.19	121.20
10	A	542	G	C6-C5-N7	-5.00	127.40	130.40
10	A	153	G	N3-C2-N2	-5.00	116.40	119.90

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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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	227	0
2	2	4529	0	4533	158	0
3	3	3466	0	3446	121	0
4	4	2111	0	2105	116	0
5	5	2624	0	2592	104	0
6	6	1738	0	1706	81	0
7	7	3110	0	3084	101	0
8	8	2919	0	2950	137	0
9	9	2867	0	2838	108	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	0	0
50	w	3308	0	3235	0	0
51	1	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	9	376	0	0	27	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	98895	1032	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 17.

All (1032) 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
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
3:3:74:ARG:NH1	3:3:140:GLU:O	2.18	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:579:LYS:NZ	5:5:71:VAL:O	2.15	0.77
1:1:402:LYS:O	1:1:406:ARG:NH1	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
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
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
9:9:520:LYS:NZ	9:9:521:ASP:O	2.19	0.73
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
9:9:444:LYS:NZ	51:9:607:HOH:O	2.17	0.71
9:9:520:LYS:NZ	51:9:608:HOH:O	2.22	0.70
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
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
1:1:572: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
1:1:107: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
8:8:336:HIS:O	8:8:344:LYS:NZ	2.27	0.62
6:6:15:LEU:HD13	6:6:45:GLU:HB3	1.79	0.62
1:1:66:LEU:HD11	1:1:151:LYS:HZ1	1.64	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
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
6:6:20:ARG:HD2	7:7:292:LYS:HZ3	1.66	0.61
1:1:159:GLN:HE22	1:1:169:ARG:HB3	1.66	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
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
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
9:9:477:GLU:OE2	9:9:479:GLN:NE2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
1:1:181:ALA:HB1	1:1:196:LYS:HZ1	1.68	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
1:1:90: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
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
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
2:2:650:LEU:HB2	2:2:653:ARG:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
1:1:222:ASN:O	1:1:225:SER:OG	2.23	0.56
3:3:50:MET:HB2	3:3:178:LEU:HD22	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:350:CYS:SG	3:3:351:ILE:N	2.79	0.55
6:6:110:GLU:CD	7:7:327:ARG:HH12	2.09	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
4:4:317:LYS:NZ	4:4:321:ASP:HA	2.21	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
1:1:558: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
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
9:9:444:LYS:NZ	51:9:669:HOH:O	2.38	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
6:6:20:ARG:HH12	7:7:295:GLU:CD	2.11	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
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
1:1:585:LEU:O	1:1:589:ARG:N	2.42	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
1:1:77:ILE:HG12	1:1:84:LYS:HZ2	1.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
9:9:303:ASN:ND2	51:9:651:HOH:O	2.42	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
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
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
1:1:414: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
9:9:211:GLU:HB2	9:9:339:LEU:HD22	1.92	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
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
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
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
1:1:580: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
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
3:3:128: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
8:8:23:LYS:HZ3	8:8:50:ASP:HB2	1.77	0.50
1:1:172:ARG:O	1:1:176:ASP:N	2.39	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
6:6:214:MET:HA	7:7:534:LYS:HZ2	1.75	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
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
1:1:13:LYS:HZ2	1:1:39:LYS:NZ	2.10	0.50
1:1:181:ALA:CB	1:1:196:LYS:HZ1	2.25	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
4:4:210:TYR:OH	4:4:216:ASN:O	2.31	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
1:1:267:PRO:HA	1:1:270:GLN:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:2:516:TYR:CZ	2:2:770:PRO:HD3	2.48	0.48
3:3:248:THR:N	3:3:289:LYS:HZ1	2.12	0.48
5:5:150:LEU:HA	5:5:166:ALA:HA	1.95	0.48
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
5:5:329:ASN:CG	7:7:537:ARG:HH12	2.17	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
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
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
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
7:7:515:SER:OG	7:7:516:ALA:N	2.45	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
3:3:172: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
6:6:16:LYS:HZ3	7:7:295:GLU:HG2	1.80	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
1:1:13:LYS:NZ	1:1:39:LYS:HZ2	2.13	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
1:1:13:LYS:HZ2	1:1:39:LYS:HZ3	1.63	0.46
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
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
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
2:2:419:PHE:O	2:2:431:LEU:N	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:336:GLN:HB3	5:5:340:LYS:HZ1	1.80	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
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
1:1:77:ILE:HG12	1:1:84:LYS:NZ	2.30	0.45
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:3:248:THR:O	3:3:289:LYS:NZ	2.48	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
1:1:110:GLN:HE21	1:1:138:GLN:HB3	1.82	0.45
1:1:354:ARG:O	1:1:357:THR:OG1	2.23	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
9:9:512:LYS:O	9:9:516:TYR:OH	2.23	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
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
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
1:1:43:TRP:HZ2	1:1:80:GLN:HB2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:3:29:LYS:HZ3	3:3:36:GLU:CD	2.21	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
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
2:2:391:THR:H	2:2:392:TYR:C	2.21	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
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
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
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
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
3:3:104:MET:HE2	3:3:141:CYS:HB2	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:9:282:LYS:O	9:9:514:GLY:N	2.44	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
3:3:108: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
3:3:311:LYS:NZ	3:3:314:GLU:OE1	2.43	0.44
4:4:179:LEU:HD21	5:5:102:GLU:HB3	2.00	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
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
2:2:583:TYR:HA	2:2:586:ARG:HE	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
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
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
2:2:393:MET:HB2	2:2:393:MET:HE3	1.91	0.43
2:2:850:THR:OG1	4:4:353:ASP:OD2	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:5:125:TYR:H	5:5:156:LYS:HZ1	1.65	0.43
5:5:276:GLN:O	5:5:280:ARG:N	2.44	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
4:4:164:ASP:OD2	4:4:205:LEU:HD11	2.17	0.43
7:7:194:PHE:HE1	7:7:232:HIS:HD1	1.66	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
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
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
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
8:8:282:PHE:CG	8:8:338:THR:HB	2.53	0.43
1:1:198:CYS:HB3	1:1:202:ARG:NH1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
8:8:103:LEU:O	8:8:107:SER:OG	2.30	0.43
9:9:195:LEU:HD23	9:9:498:TRP:HB3	2.00	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
4:4:317:LYS:HZ3	4:4:321:ASP:HA	1.82	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
9:9:526:MET:SD	9:9:528:ARG:NH2	2.92	0.42
1:1:73: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
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
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
1:1:342: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:4:232:SER:HB3	5:5:220:LYS:HZ3	1.84	0.42
4:4:347:LEU:O	4:4:351:ILE:N	2.41	0.42
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
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
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
8:8:143:GLU:OE2	8:8:161:LYS:NZ	2.52	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
6:6:20:ARG:CZ	7:7:292:LYS:HZ1	2.33	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:3:35:LYS:HZ1	3:3:322:ASP:HA	1.84	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
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
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
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
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
2:2:503:TYR:HH	2:2:572:HIS:HE2	1.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
2:2:434: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
5:5:216:TRP:CE2	5:5:220:LYS:NZ	2.87	0.40
7:7:487:ARG:HA	7:7:488:ILE:HA	1.76	0.40
8:8:335:SER:O	8:8:335:SER:OG	2.38	0.40
9:9:371:ARG:HB2	9:9:373:TRP:CH2	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
8:8:61:GLU:HG2	8:8:98:ARG:HH12	1.87	0.40
1:1:13:LYS:HZ1	1:1:39:LYS:HZ2	1.69	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
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
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%)	44	78
2	2	556/843 (66%)	507 (91%)	48 (9%)	1 (0%)	44	78
3	3	418/445 (94%)	348 (83%)	64 (15%)	6 (1%)	9	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	37	72
8	8	364/374 (97%)	301 (83%)	63 (17%)	0	100	100
9	9	350/368 (95%)	325 (93%)	23 (7%)	2 (1%)	22	60
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%)	12	47
15	J	51/53 (96%)	46 (90%)	5 (10%)	0	100	100
16	K	180/182 (99%)	165 (92%)	14 (8%)	1 (1%)	22	60
17	L	135/137 (98%)	114 (84%)	21 (16%)	0	100	100
19	P	264/266 (99%)	212 (80%)	48 (18%)	4 (2%)	8	40
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%)	25	64
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	55
34	f	206/208 (99%)	177 (86%)	27 (13%)	2 (1%)	13	49
35	g	225/227 (99%)	203 (90%)	20 (9%)	2 (1%)	14	51
36	h	102/104 (98%)	94 (92%)	8 (8%)	0	100	100
37	i	213/215 (99%)	188 (88%)	25 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	j	134/136 (98%)	117 (87%)	16 (12%)	1 (1%)	19	57
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%)	8	38
43	o	204/206 (99%)	173 (85%)	29 (14%)	2 (1%)	13	49
44	p	69/71 (97%)	48 (70%)	21 (30%)	0	100	100
45	q	235/237 (99%)	211 (90%)	22 (9%)	2 (1%)	14	51
46	r	122/124 (98%)	97 (80%)	23 (19%)	2 (2%)	8	38
47	s	129/131 (98%)	110 (85%)	18 (14%)	1 (1%)	16	55
48	t	96/98 (98%)	76 (79%)	19 (20%)	1 (1%)	13	49
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%)	27	64

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
46	r	118	SER
3	3	238	TYR

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Mol	Chain	Res	Type
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 ⓘ

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%)	542 (98%)	9 (2%)	58	73
2	2	503/750 (67%)	497 (99%)	6 (1%)	67	79
3	3	384/406 (95%)	371 (97%)	13 (3%)	32	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	4	239/282 (85%)	234 (98%)	5 (2%)	48	66
5	5	293/311 (94%)	287 (98%)	6 (2%)	50	68
6	6	190/193 (98%)	189 (100%)	1 (0%)	86	89
7	7	342/516 (66%)	340 (99%)	2 (1%)	84	88
8	8	327/335 (98%)	327 (100%)	0	100	100
9	9	320/331 (97%)	317 (99%)	3 (1%)	75	83
12	G	142/142 (100%)	137 (96%)	5 (4%)	31	51
13	H	117/117 (100%)	114 (97%)	3 (3%)	41	59
14	I	225/225 (100%)	222 (99%)	3 (1%)	65	77
15	J	47/47 (100%)	47 (100%)	0	100	100
16	K	157/157 (100%)	156 (99%)	1 (1%)	84	88
17	L	119/119 (100%)	118 (99%)	1 (1%)	79	85
19	P	238/238 (100%)	231 (97%)	7 (3%)	37	56
20	Q	114/114 (100%)	113 (99%)	1 (1%)	75	83
21	R	113/113 (100%)	111 (98%)	2 (2%)	54	71
22	S	354/354 (100%)	349 (99%)	5 (1%)	62	75
23	U	161/161 (100%)	157 (98%)	4 (2%)	42	61
24	V	49/49 (100%)	48 (98%)	1 (2%)	50	68
25	W	66/66 (100%)	66 (100%)	0	100	100
26	X	170/170 (100%)	168 (99%)	2 (1%)	67	79
27	Y	76/76 (100%)	75 (99%)	1 (1%)	65	77
28	Z	130/130 (100%)	130 (100%)	0	100	100
29	a	112/112 (100%)	111 (99%)	1 (1%)	75	83
30	b	67/67 (100%)	65 (97%)	2 (3%)	36	55
31	c	187/187 (100%)	186 (100%)	1 (0%)	86	89
32	d	17/17 (100%)	17 (100%)	0	100	100
33	e	114/114 (100%)	112 (98%)	2 (2%)	54	71
34	f	174/174 (100%)	170 (98%)	4 (2%)	45	64
35	g	190/190 (100%)	188 (99%)	2 (1%)	70	80
36	h	94/94 (100%)	94 (100%)	0	100	100
37	i	196/196 (100%)	195 (100%)	1 (0%)	86	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	j	106/106 (100%)	105 (99%)	1 (1%)	75	83
39	k	87/87 (100%)	84 (97%)	3 (3%)	32	51
40	l	57/57 (100%)	56 (98%)	1 (2%)	54	71
41	m	272/272 (100%)	270 (99%)	2 (1%)	81	87
42	n	116/116 (100%)	112 (97%)	4 (3%)	32	51
43	o	177/177 (100%)	174 (98%)	3 (2%)	56	72
44	p	64/64 (100%)	64 (100%)	0	100	100
45	q	207/207 (100%)	205 (99%)	2 (1%)	73	82
46	r	104/104 (100%)	104 (100%)	0	100	100
47	s	113/113 (100%)	112 (99%)	1 (1%)	75	83
48	t	89/89 (100%)	88 (99%)	1 (1%)	70	80
49	u	66/548 (12%)	61 (92%)	5 (8%)	11	30
50	w	360/928 (39%)	358 (99%)	2 (1%)	84	88
All	All	8396/10666 (79%)	8277 (99%)	119 (1%)	62	75

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	16	ASN
1	1	76	ASN
1	1	110	GLN
1	1	274	ASN
1	1	309	ASN
1	1	321	ARG
1	1	434	ASN
1	1	521	ASN
1	1	575	ILE
2	2	340	ARG
2	2	371	ILE
2	2	560	ARG
2	2	615	GLN
2	2	658	ARG
2	2	678	ASN
3	3	26	LEU
3	3	38	LEU
3	3	94	MET
3	3	97	ASP

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Mol	Chain	Res	Type
3	3	133	ARG
3	3	143	ASN
3	3	163	ARG
3	3	193	LYS
3	3	224	ASN
3	3	229	ARG
3	3	270	ARG
3	3	361	ASN
3	3	375	ILE
4	4	115	HIS
4	4	140	LEU
4	4	280	ASN
4	4	322	ASN
4	4	350	ASN
5	5	168	ARG
5	5	197	MET
5	5	237	ASN
5	5	285	ASN
5	5	351	ASN
5	5	352	ASN
6	6	10	ASN
7	7	296	ASN
7	7	527	MET
9	9	189	ARG
9	9	291	LYS
9	9	496	ASN
12	G	8	ARG
12	G	58	LYS
12	G	69	ARG
12	G	101	ARG
12	G	141	ASN
13	H	37	ARG
13	H	105	LYS
13	H	131	LYS
14	I	49	ARG
14	I	113	ARG
14	I	216	ASN
16	K	172	ARG
17	L	118	ARG
19	P	7	ARG
19	P	23	ASN
19	P	30	MET

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Mol	Chain	Res	Type
19	P	41	ASN
19	P	45	MET
19	P	113	ARG
19	P	179	ASN
20	Q	3	LYS
21	R	28	LEU
21	R	75	MET
22	S	89	ASN
22	S	203	ASN
22	S	242	LYS
22	S	284	VAL
22	S	453	LYS
23	U	55	ARG
23	U	81	ARG
23	U	130	ARG
23	U	165	ASN
24	V	82	ARG
26	X	12	ASN
26	X	33	ASN
27	Y	33	MET
29	a	5	ASN
30	b	4	ASN
30	b	47	ASN
31	c	61	LYS
33	e	3	ARG
33	e	67	ARG
34	f	149	ASN
34	f	164	ASN
34	f	186	ARG
34	f	191	ARG
35	g	94	ARG
35	g	178	ARG
37	i	76	ASN
38	j	66	ARG
39	k	5	ARG
39	k	51	ARG
39	k	85	ARG
40	l	32	VAL
41	m	100	ARG
41	m	245	ARG
42	n	51	ARG
42	n	72	LYS

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Mol	Chain	Res	Type
42	n	81	ARG
42	n	100	LYS
43	o	64	ASN
43	o	84	ASN
43	o	140	LYS
45	q	67	VAL
45	q	131	ARG
47	s	61	ARG
48	t	95	ARG
49	u	13	THR
49	u	22	ARG
49	u	31	LEU
49	u	37	ASN
49	u	44	PHE
50	w	453	ARG
50	w	500	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) 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	159	GLN
1	1	180	GLN
1	1	207	GLN
1	1	212	HIS
1	1	229	HIS
1	1	236	GLN
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	481	GLN
1	1	512	GLN
2	2	355	GLN
2	2	377	ASN

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Mol	Chain	Res	Type
2	2	386	ASN
2	2	460	GLN
2	2	487	GLN
2	2	610	ASN
2	2	678	ASN
2	2	716	HIS
2	2	717	GLN
2	2	736	HIS
2	2	753	HIS
2	2	758	ASN
2	2	762	ASN
3	3	12	HIS
3	3	17	HIS
3	3	49	ASN
3	3	143	ASN
3	3	224	ASN
3	3	231	ASN
3	3	264	ASN
3	3	302	ASN
3	3	321	ASN
3	3	335	ASN
3	3	361	ASN
3	3	390	HIS
4	4	130	ASN
4	4	147	HIS
4	4	322	ASN
4	4	333	ASN
4	4	350	ASN
5	5	111	ASN
5	5	191	ASN
5	5	212	ASN
5	5	237	ASN
5	5	273	GLN
5	5	285	ASN
5	5	336	GLN
5	5	345	GLN
5	5	351	ASN
6	6	10	ASN
6	6	93	HIS
6	6	186	GLN
7	7	195	GLN
7	7	223	ASN

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Mol	Chain	Res	Type
7	7	225	HIS
7	7	229	ASN
7	7	281	HIS
7	7	289	GLN
7	7	368	HIS
7	7	436	HIS
7	7	443	GLN
7	7	453	GLN
7	7	454	GLN
7	7	548	HIS
8	8	111	HIS
8	8	270	HIS
8	8	327	GLN
8	8	345	GLN
8	8	359	GLN
9	9	303	ASN
9	9	479	GLN
49	u	37	ASN
50	w	414	ASN
50	w	500	ASN
50	w	513	GLN
50	w	582	ASN

5.3.3 RNA ⓘ

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

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Mol	Chain	Res	Type
10	A	33	G
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

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Mol	Chain	Res	Type
10	A	135	U
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

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Mol	Chain	Res	Type
10	A	223	A
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

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Mol	Chain	Res	Type
10	A	335	U
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

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Mol	Chain	Res	Type
10	A	466	A
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

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Mol	Chain	Res	Type
10	A	548	G
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

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Mol	Chain	Res	Type
10	A	640	A
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

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Mol	Chain	Res	Type
10	A	808	A
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

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Mol	Chain	Res	Type
10	A	906	G
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

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Mol	Chain	Res	Type
10	A	1028	C
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

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Mol	Chain	Res	Type
10	A	1139	A
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

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Mol	Chain	Res	Type
10	A	1289	A
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

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Mol	Chain	Res	Type
10	A	1407	G
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

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Mol	Chain	Res	Type
10	A	1502	A
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

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Mol	Chain	Res	Type
10	A	1596	A
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

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Mol	Chain	Res	Type
10	A	1724	U
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

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Mol	Chain	Res	Type
10	A	1804	U
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

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Mol	Chain	Res	Type
18	N	8	U
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

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Mol	Chain	Res	Type
10	A	455	A
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 ⓘ

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

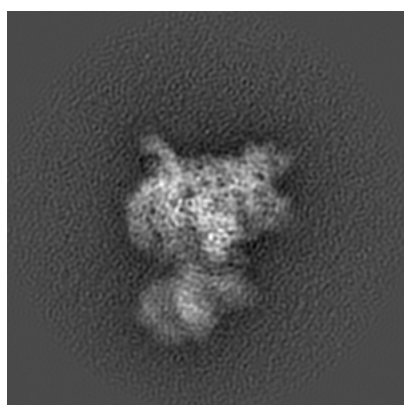
6 Map visualisation [i](#)

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.

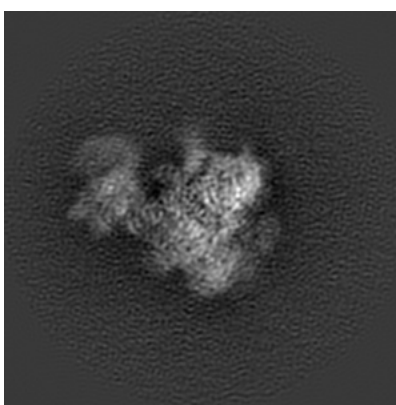
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

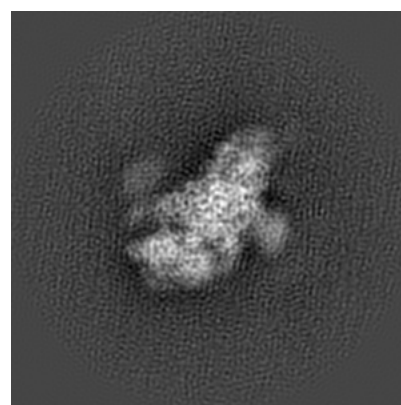
6.1.1 Primary map



X



Y

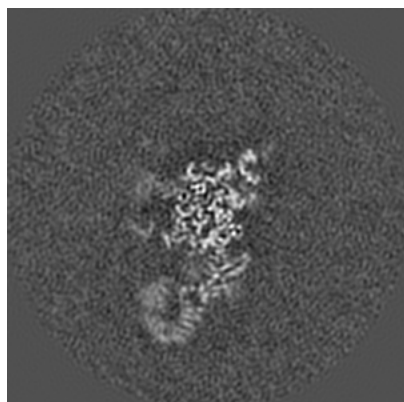


Z

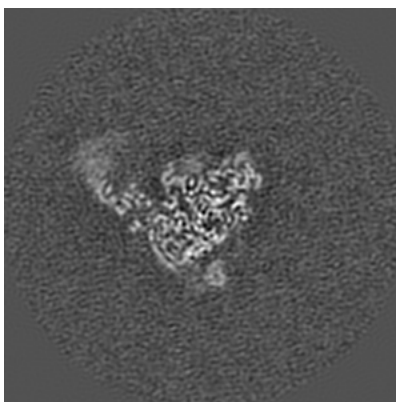
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

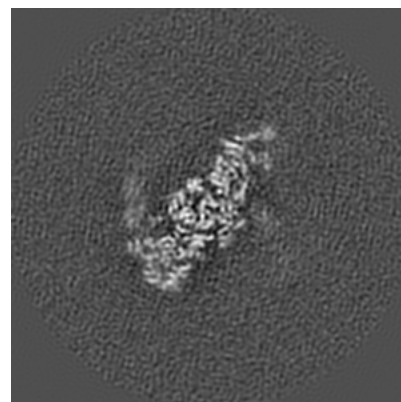
6.2.1 Primary map



X Index: 104



Y Index: 104

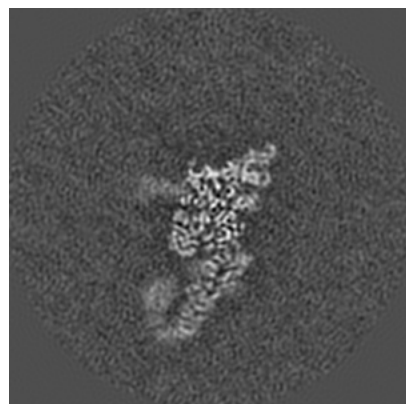


Z Index: 104

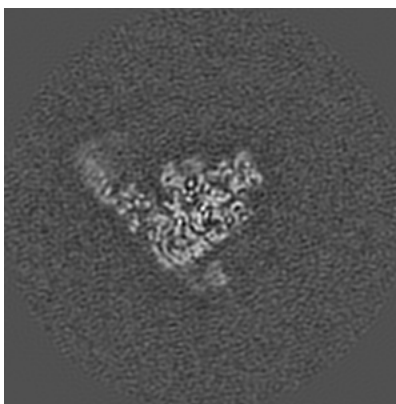
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

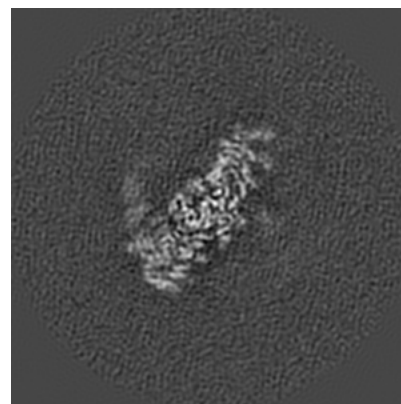
6.3.1 Primary map



X Index: 106



Y Index: 105

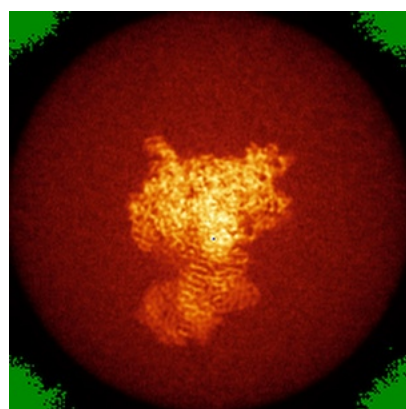


Z Index: 105

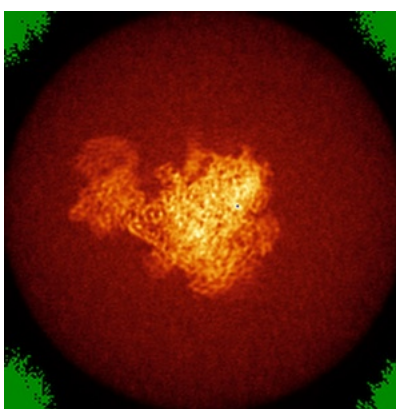
The images above show the largest variance slices of the map in three orthogonal directions.

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

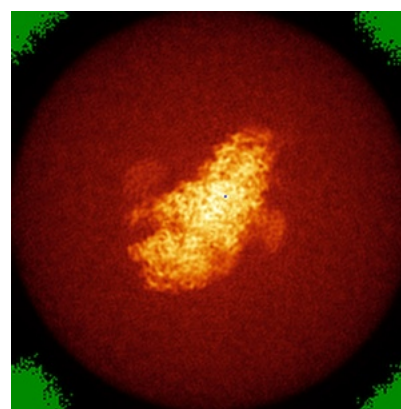
6.4.1 Primary map



X



Y

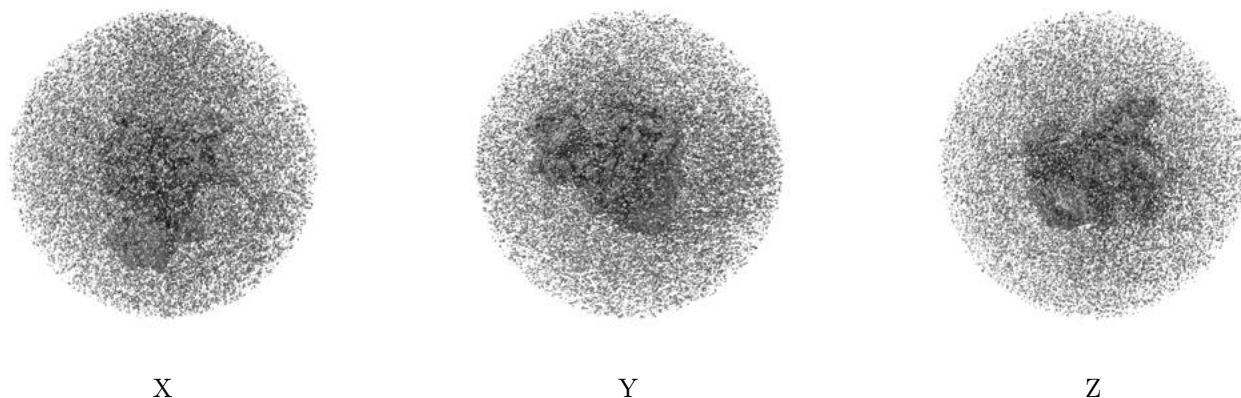


Z

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 [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

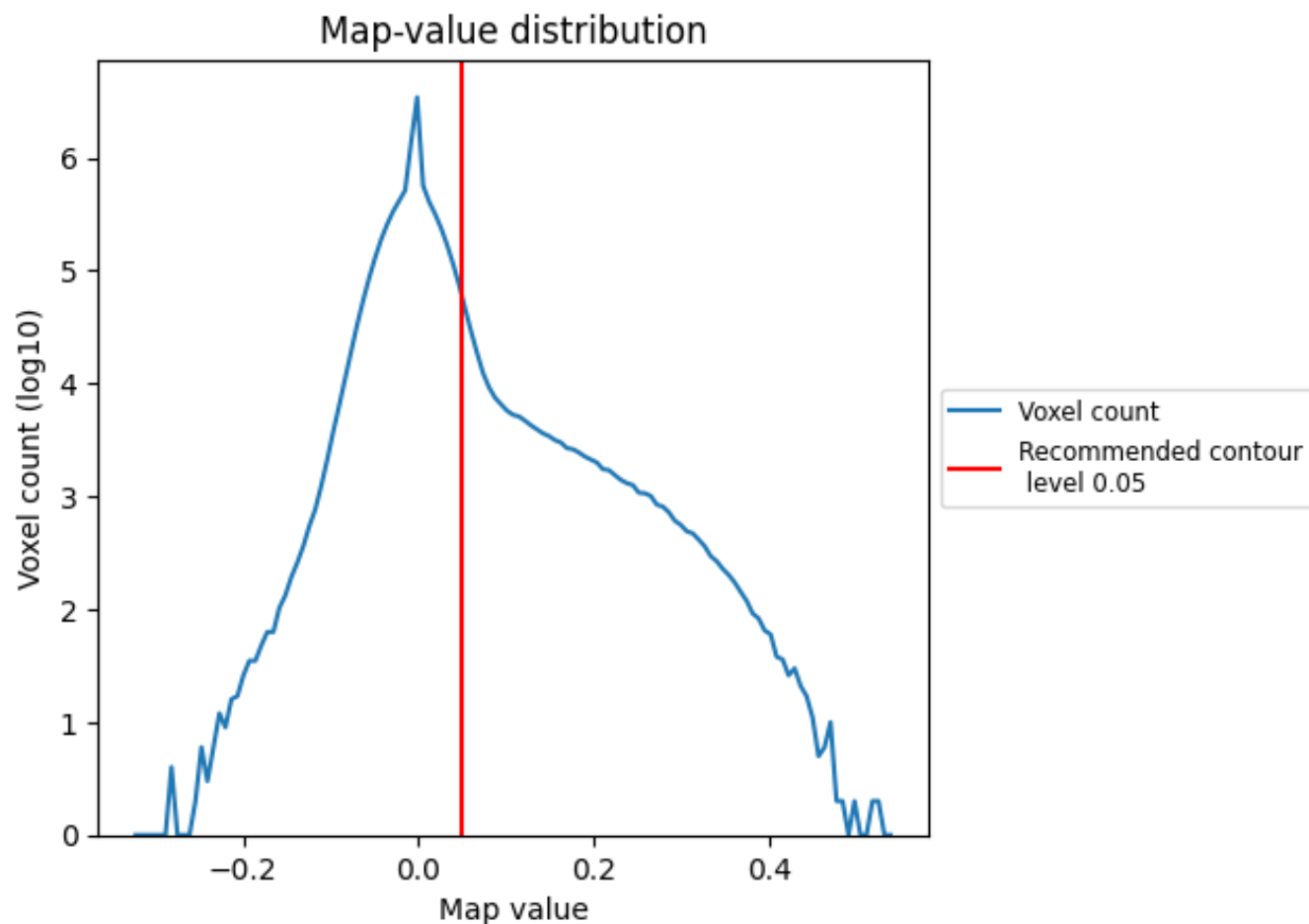
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

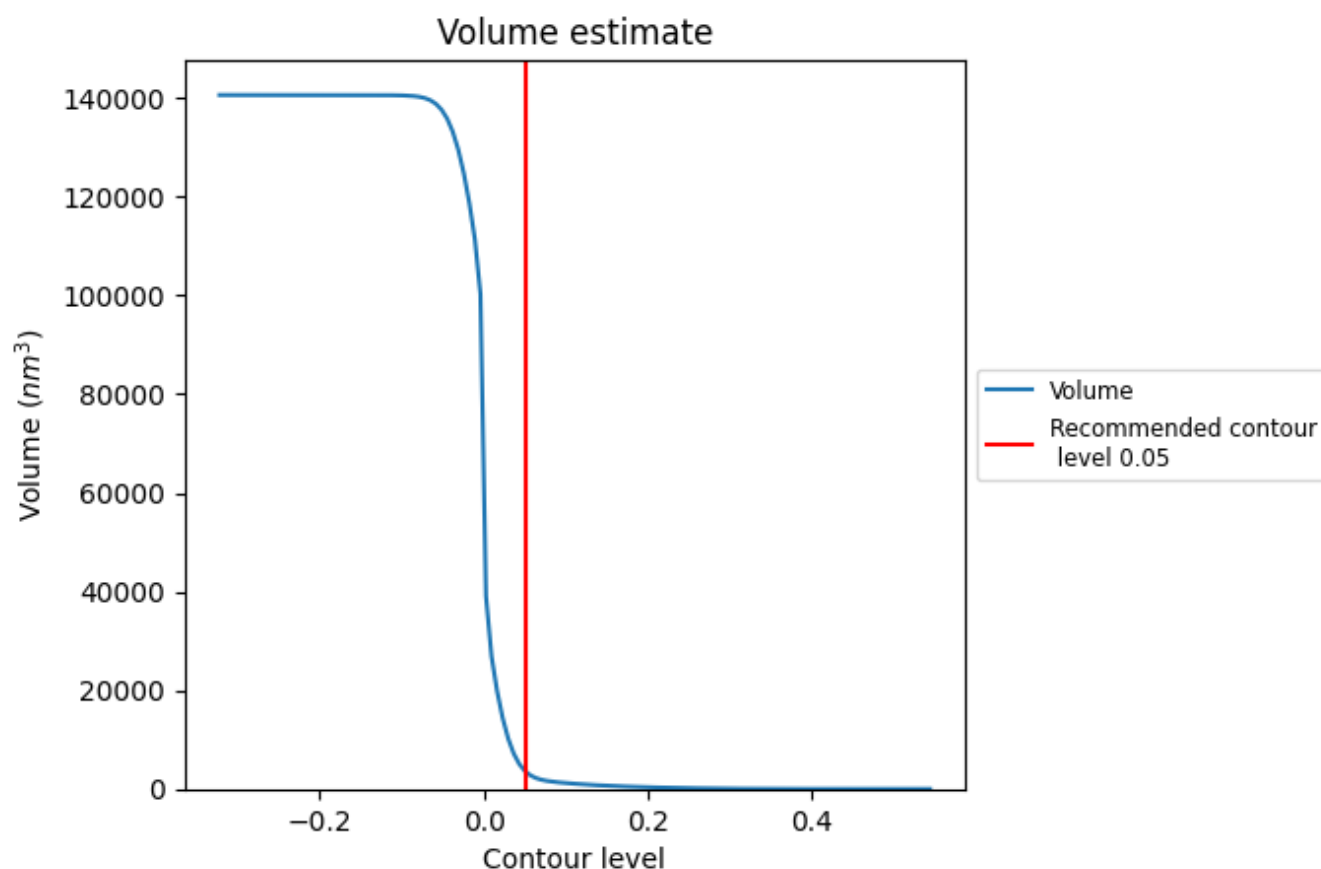
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

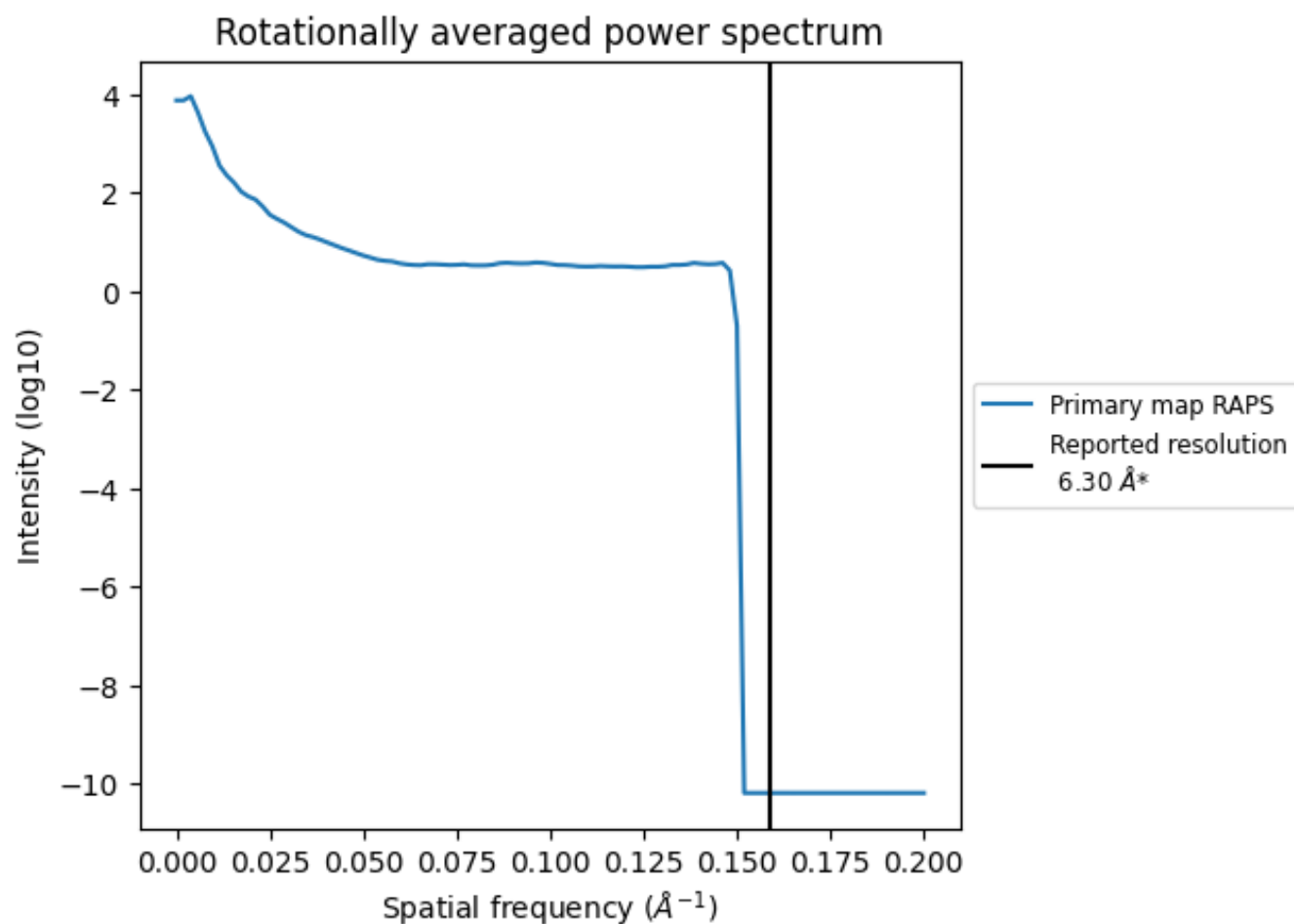
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3639 nm³; 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.159 \AA^{-1}

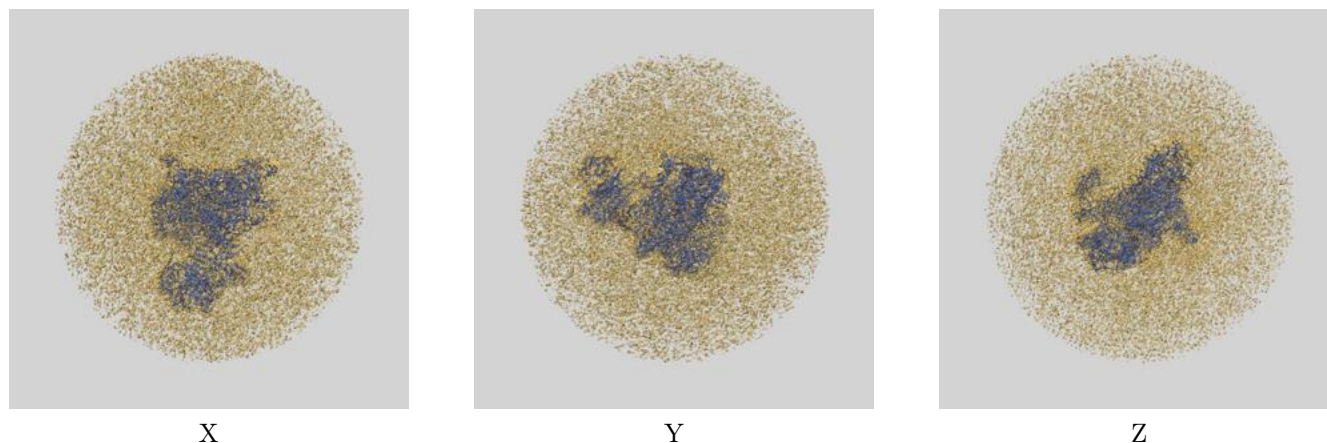
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

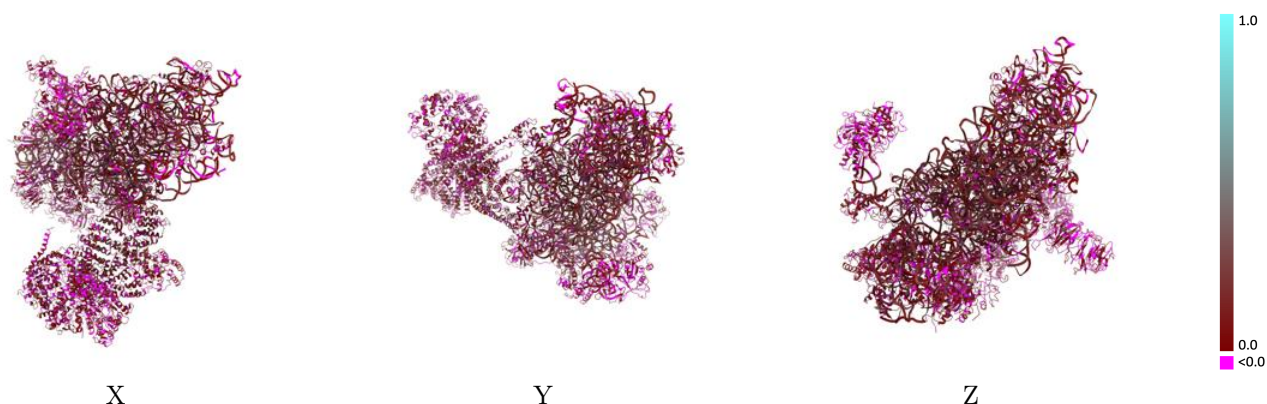
This section contains information regarding the fit between EMDB map EMD-4242 and PDB model 6FEC. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



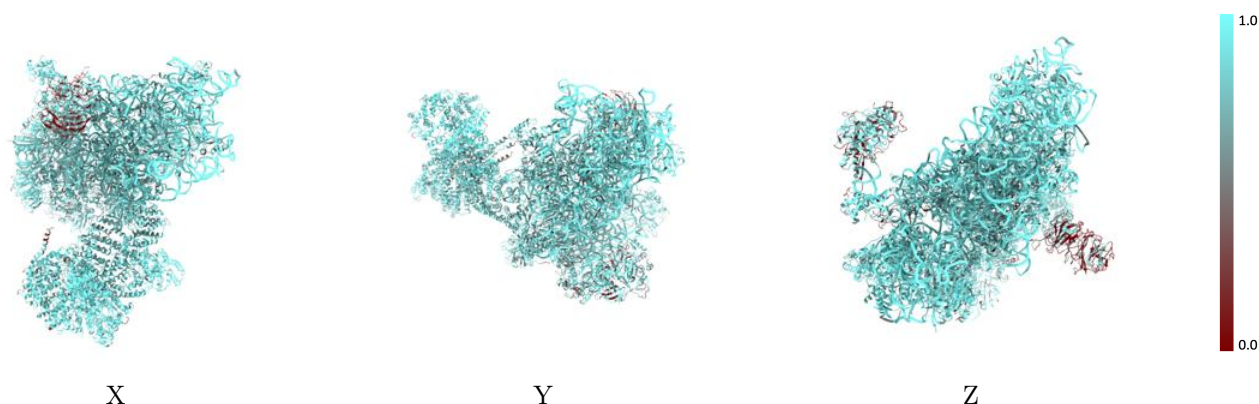
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



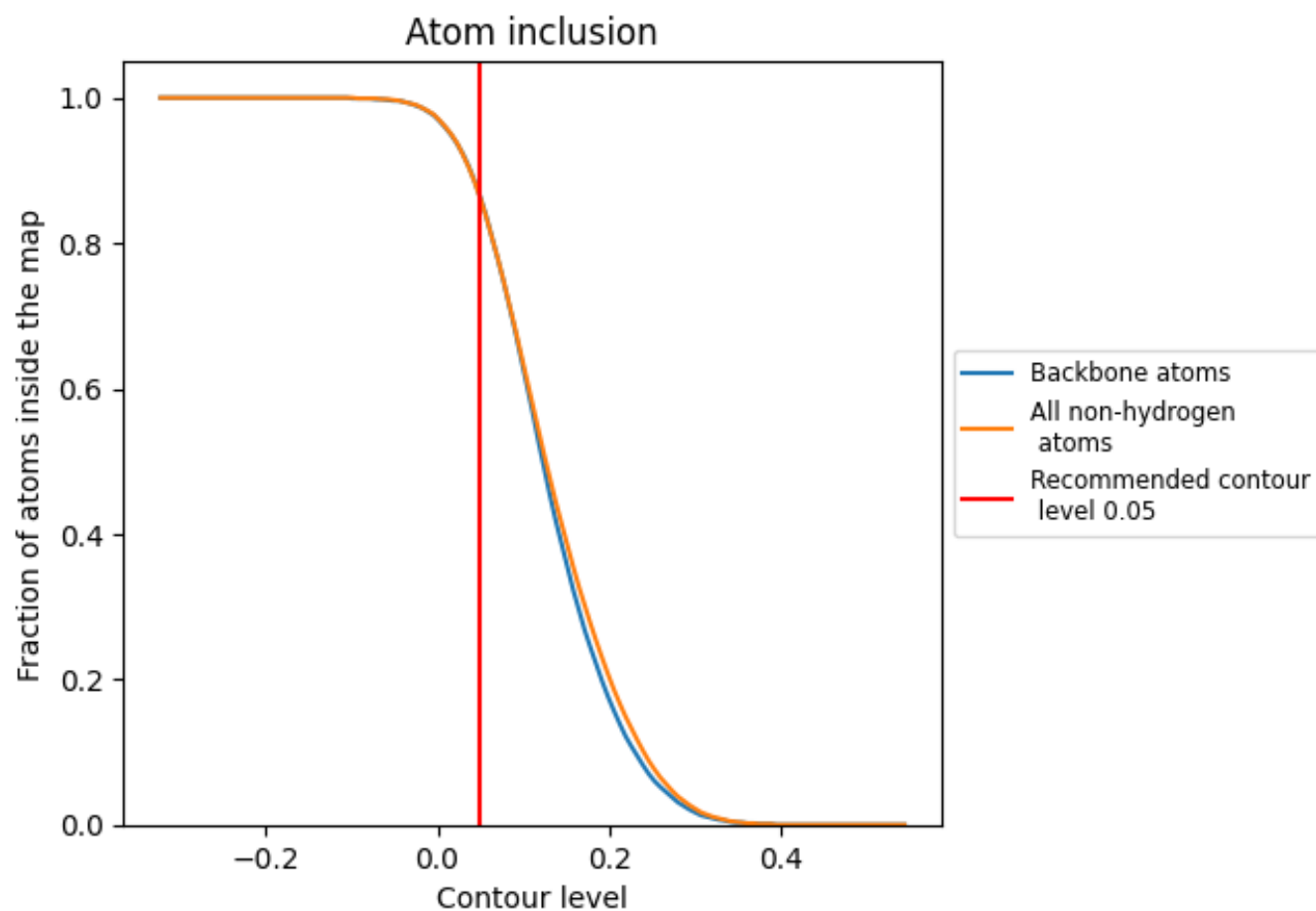
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).







































































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