



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 02:50 PM UTC

PDB ID : 8AGX / pdb_00008agx
EMDB ID : EMD-15427
Title : Yeast RQC complex in state with the RING domain of Ltn1 in the IN position
Authors : Tesina, P.; Buschauer, R.; Beckmann, R.
Deposited on : 2022-07-20
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

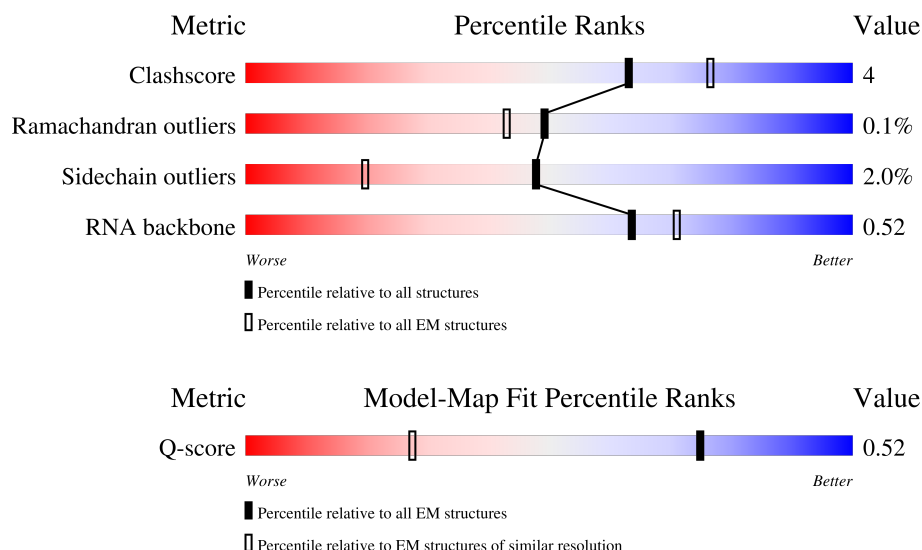
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.40 Å.

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



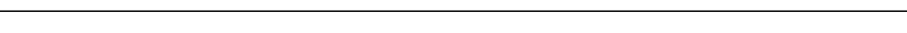
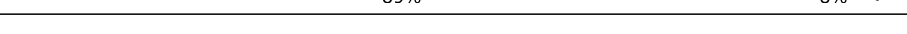
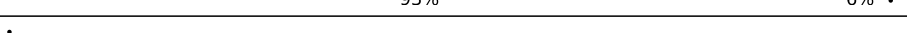
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	5628 (1.90 - 2.90)

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	A	204	 88% 12%
2	B	199	 85% 14% .
3	C	184	 84% 15% ..

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Mol	Chain	Length	Quality of chain
4	D	186	
5	E	189	
6	F	172	
7	G	160	
8	H	121	
9	I	137	
10	J	155	
11	K	142	
12	L	127	
13	M	136	
14	N	149	
15	O	59	
16	P	105	
17	Q	113	
18	R	130	
19	S	107	
20	T	121	
21	U	120	
22	V	100	
23	W	88	
24	X	78	
25	Y	51	
26	Z	128	
27	b	106	
28	c	92	

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Mol	Chain	Length	Quality of chain
29	d	25	
30	f	3395	
31	h	121	
32	i	158	
33	j	254	
34	k	387	
35	l	362	
36	m	297	
37	n	176	
38	o	244	
39	p	256	
40	q	191	
41	r	221	
42	s	174	
43	t	199	
44	u	138	
45	a	1038	
46	e	1562	
47	v	157	
48	w	217	
49	x	76	
49	y	76	
50	z	165	
51	0	312	
52	1	18	

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 149706 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 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 2 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	197	Total	C	N	O	S	197	0
			1555	1003	289	262	1		

- Molecule 3 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	183	Total	C	N	O		0	0
			1416	879	284	253			

- Molecule 4 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	185	Total	C	N	O	S	0	0
			1441	908	290	241	2		

- Molecule 5 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	156	Total	C	N	O		0	0
			1258	781	265	212			

- Molecule 6 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	171	Total	C	N	O	S	0	0
			1437	925	266	243	3		

- Molecule 7 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	159	Total	C	N	O	S	0	0
			1272	802	245	221	4		

- Molecule 8 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	102	Total	C	N	O	S	0	0
			812	526	134	152			

- Molecule 9 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	136	Total	C	N	O	S	0	0
			1003	628	189	179	7		

- Molecule 10 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	63	Total	C	N	O	S	0	0
			518	333	102	82	1		

- Molecule 11 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	121	Total	C	N	O	S	0	0
			964	620	169	173	2		

- Molecule 12 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	125	Total	C	N	O	S	0	0
			984	620	191	173			

- Molecule 13 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	135	Total	C	N	O	S	0	0
			1080	701	199	180			

- Molecule 14 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	148	Total	C	N	O	S	0	0
			1169	747	231	188	3		

- Molecule 15 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	58	Total	C	N	O	S	0	0
			462	289	100	73			

- Molecule 16 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	96	Total	C	N	O	S	0	0
			737	476	123	137	1		

- Molecule 17 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	109	Total	C	N	O	S	0	0
			876	556	167	152	1		

- Molecule 18 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	127	Total	C	N	O	S	0	0
			1013	642	205	165	1		

- Molecule 19 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 20 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	112	Total	C	N	O	S	0	0
			880	545	179	152	4		

- Molecule 21 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 22 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	99	Total	C	N	O	S	0	0
			766	478	154	132	2		

- Molecule 23 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	81	Total	C	N	O	S	0	0
			645	393	141	106	5		

- Molecule 24 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	77	Total	C	N	O		0	0
			612	391	115	106			

- Molecule 25 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 26 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	52	Total	C	N	O	S	0	0
			410	254	86	65	5		

- Molecule 27 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	103	Total	C	N	O	S	0	0
			824	517	167	135	5		

- Molecule 28 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 29 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	22	Total	C	N	O	S	0	0
			207	127	56	23	1		

- Molecule 30 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	f	3216	Total	C	N	O	P	0	0
			68782	30723	12389	22454	3216		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
f	?	-	G	deletion	GB 2211412835
f	1956	U	-	insertion	GB 2211412835
f	?	-	A	deletion	GB 2211412835
f	2255	U	-	insertion	GB 2211412835
f	?	-	G	deletion	GB 2211412835

- Molecule 31 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 32 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	i	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 33 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	j	246	Total	C	N	O	S	0	0
			1874	1168	380	325	1		

- Molecule 34 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	k	386	Total	C	N	O	S	0	0
			3075	1950	584	533	8		

- Molecule 35 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	l	361	Total	C	N	O	S	0	0
			2748	1729	522	494	3		

- Molecule 36 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	294	Total	C	N	O	S	0	0
			2351	1484	410	455	2		

- Molecule 37 is a protein called 60S ribosomal protein L6-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	n	167	Total	C	N	O		0	0
			1307	843	234	230			

- Molecule 38 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	o	222	Total	C	N	O	S	0	0
			1784	1151	324	308	1		

- Molecule 39 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	p	233	Total	C	N	O	S	0	0
			1804	1151	323	327	3		

- Molecule 40 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	q	191	Total	C	N	O	S	0	0
			1508	957	274	273	4		

- Molecule 41 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	r	218	Total	C	N	O	S	0	0
			1764	1117	334	306	7		

- Molecule 42 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	s	169	Total	C	N	O	S	0	0
			1346	843	252	247	4		

- Molecule 43 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	t	193	Total	C	N	O	S	0	0
			1543	962	315	266			

- Molecule 44 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	u	136	Total	C	N	O	S	0	0
			1053	675	199	177	2		

- Molecule 45 is a protein called Ribosome quality control complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	a	848	Total	C	N	O	S	0	0
			6579	4194	1142	1226	17		

- Molecule 46 is a protein called E3 ubiquitin-protein ligase listerin.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	e	1527	Total	C	N	O	S	0	0
			11508	7354	1936	2180	38		

- Molecule 47 is a protein called Eukaryotic translation initiation factor 5A-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	v	142	Total	C	N	O	S	0	0
			1085	676	183	217	9		

- Molecule 48 is a protein called 60S ribosomal protein L1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	w	216	Total	C	N	O	S	0	0
			1709	1092	298	310	9		

- Molecule 49 is a RNA chain called Ala tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	x	74	Total	C	N	O	P	0	0
			1579	702	277	526	74		
49	y	73	Total	C	N	O	P	0	0
			1556	692	272	519	73		

- Molecule 50 is a protein called 60S ribosomal protein L12-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	z	148	Total	C	N	O	0	0
			728	432	148	148		

- Molecule 51 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	0	121	Total	C	N	O	S	0	0
			961	618	167	173	3		

- Molecule 52 is a protein called CAT-tailed nascent peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	1	18	Total	C	N	O	0	0
			90	54	18	18		

- Molecule 53 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
53	A	1	Total	Mg	0
			1	1	
53	C	1	Total	Mg	0
			1	1	
53	E	1	Total	Mg	0
			1	1	
53	I	1	Total	Mg	0
			1	1	
53	R	1	Total	Mg	0
			1	1	

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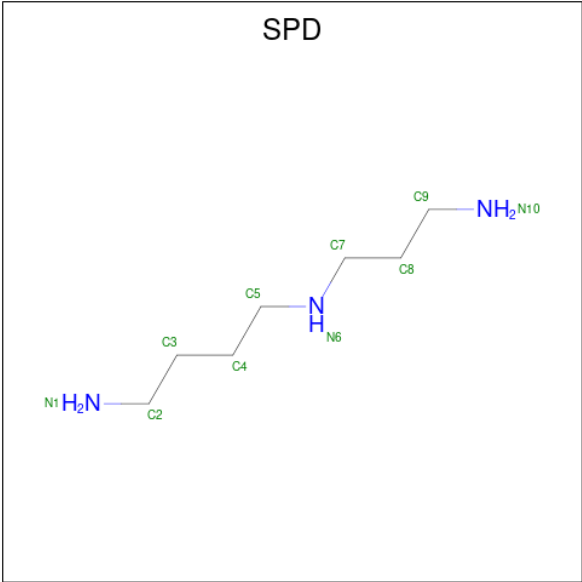
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Mol	Chain	Residues	Atoms		AltConf
53	T	1	Total 1	Mg 1	0
53	f	3	Total 3	Mg 3	0
53	h	1	Total 1	Mg 1	0
53	j	2	Total 2	Mg 2	0
53	k	1	Total 1	Mg 1	0

- Molecule 54 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
54	T	1	Total 1	Zn 1	0
54	W	1	Total 1	Zn 1	0
54	Z	1	Total 1	Zn 1	0
54	b	1	Total 1	Zn 1	0
54	c	1	Total 1	Zn 1	0
54	e	2	Total 2	Zn 2	0

- Molecule 55 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃).

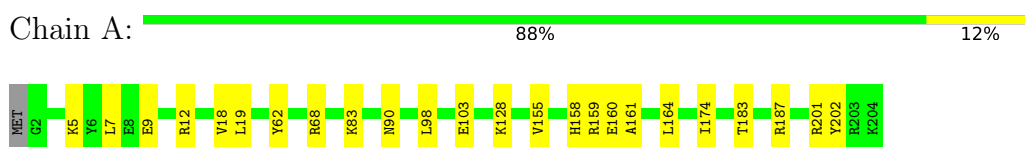


Mol	Chain	Residues	Atoms			AltConf
55	f	1	Total	C	N	0
			10	7	3	

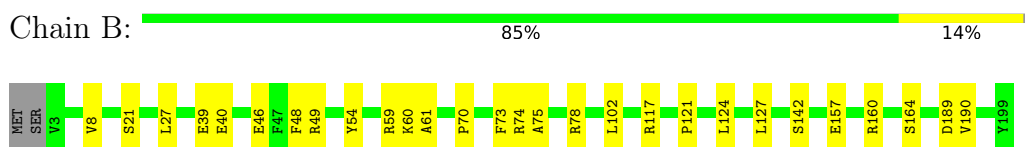
3 Residue-property plots [i](#)

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

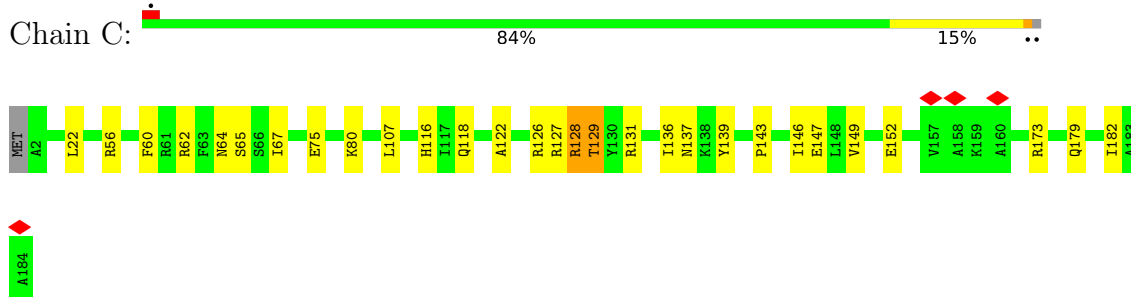
- Molecule 1: 60S ribosomal protein L15-A



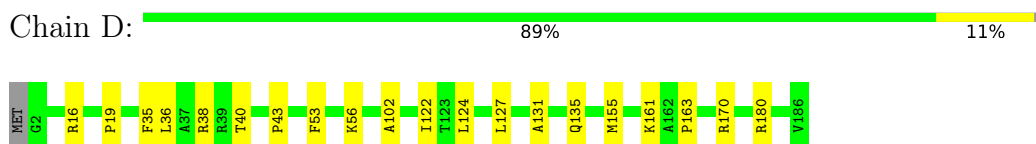
- Molecule 2: 60S ribosomal protein L16-A



- Molecule 3: 60S ribosomal protein L17-A

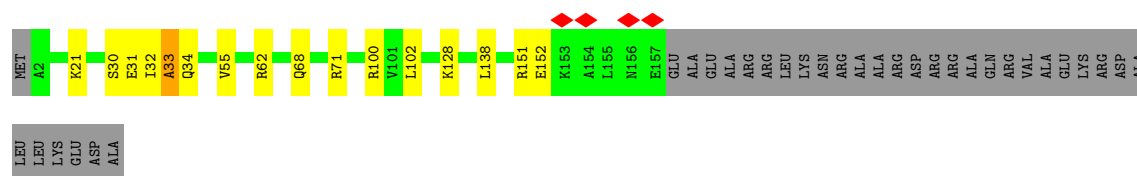


- Molecule 4: 60S ribosomal protein L18-A



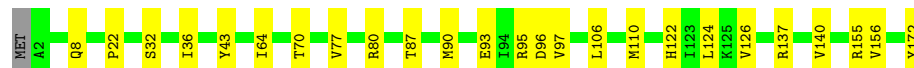
- Molecule 5: 60S ribosomal protein L19-A





- Molecule 6: 60S ribosomal protein L20-A

Chain F: 85% 15%



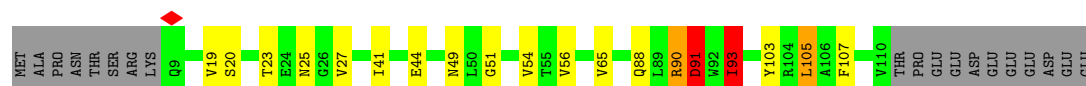
- Molecule 7: 60S ribosomal protein L21-A

Chain G: 87% 12%



- Molecule 8: 60S ribosomal protein L22-A

Chain H: 69% 12% 16%



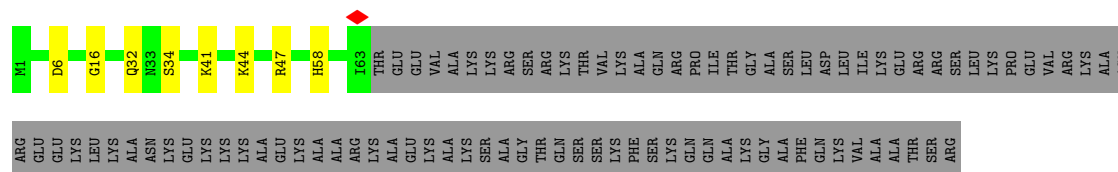
- Molecule 9: 60S ribosomal protein L23-A

Chain I: 89% 10%



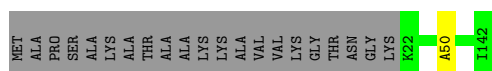
- Molecule 10: 60S ribosomal protein L24-A

Chain J: 35% 5% 59%



- Molecule 11: 60S ribosomal protein L25

Chain K: 85% 15%



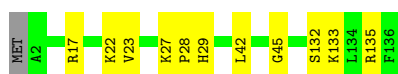
- Molecule 12: 60S ribosomal protein L26-A

Chain L: 91% 8% .



- Molecule 13: 60S ribosomal protein L27-A

Chain M: 91% 8% .



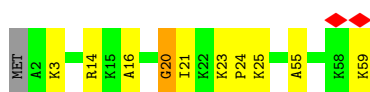
- Molecule 14: 60S ribosomal protein L28

Chain N: 87% 13% .



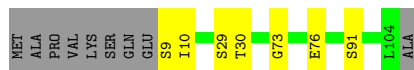
- Molecule 15: 60S ribosomal protein L29

Chain O: 81% 15% . .



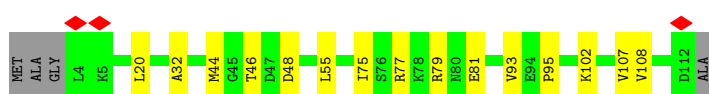
- Molecule 16: 60S ribosomal protein L30

Chain P: 85% 7% 9%



- Molecule 17: 60S ribosomal protein L31-A

Chain Q: 83% 13% .



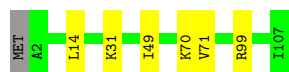
- Molecule 18: 60S ribosomal protein L32

Chain R: 89% 8% .



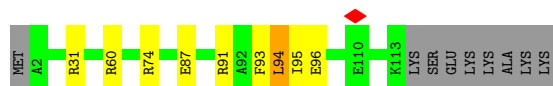
- Molecule 19: 60S ribosomal protein L33-A

Chain S: 93% 6%



- Molecule 20: 60S ribosomal protein L34-A

Chain T: 85% 7% 7%



- Molecule 21: 60S ribosomal protein L35-A

Chain U: 92% 7%



- Molecule 22: 60S ribosomal protein L36-A

Chain V: 90% 9%



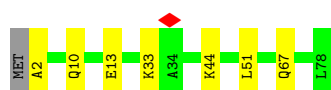
- Molecule 23: 60S ribosomal protein L37-A

Chain W: 76% 16% 8%



- Molecule 24: 60S ribosomal protein L38

Chain X: 90% 9%

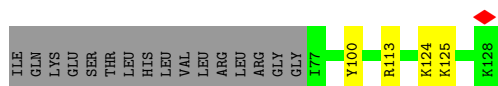
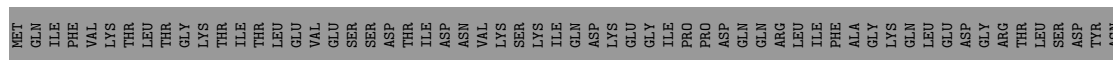


- Molecule 25: 60S ribosomal protein L39

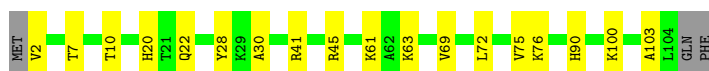
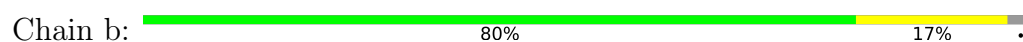
Chain Y: 92% 6%



- Molecule 26: Ubiquitin-60S ribosomal protein L40



- Molecule 27: 60S ribosomal protein L42-A



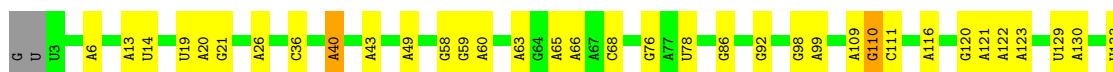
- Molecule 28: 60S ribosomal protein L43-A



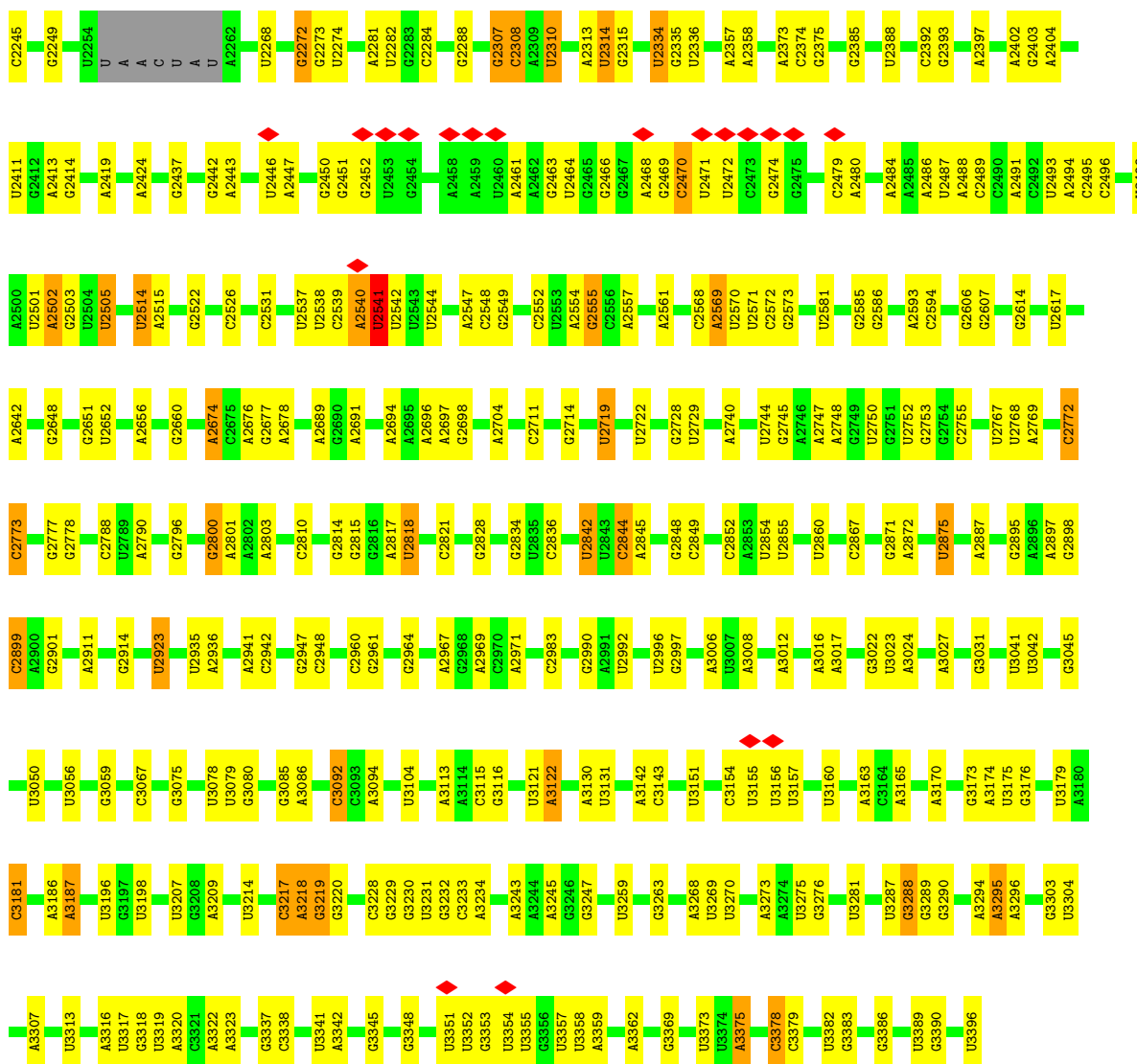
- Molecule 29: 60S ribosomal protein L41-A



- Molecule 30: 25S rRNA

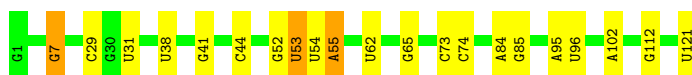






- Molecule 31: 5S rRNA

Chain h: 83% 15% .



- Molecule 32: 5.8S rRNA

Chain i: 73% 23% .



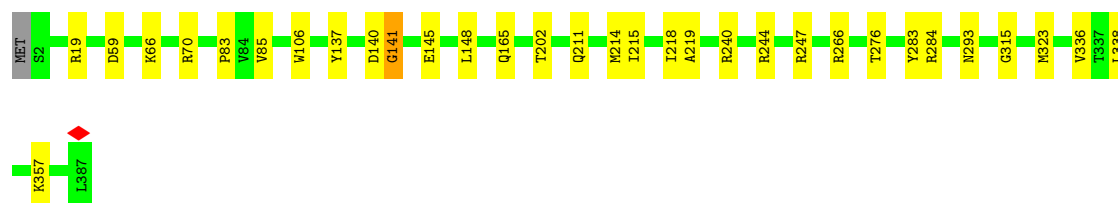
- Molecule 33: 60S ribosomal protein L2-A

Chain j:  84% 13%



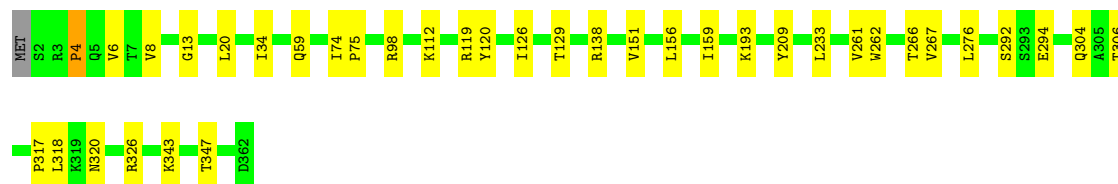
- Molecule 34: 60S ribosomal protein L3

Chain k:  91% 8%



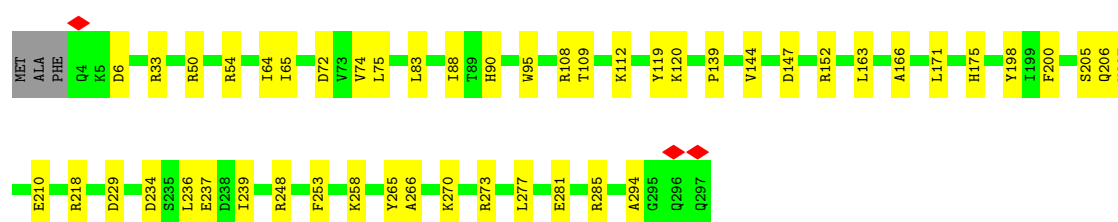
- Molecule 35: 60S ribosomal protein L4-A

Chain l:  90% 10%



- Molecule 36: 60S ribosomal protein L5

Chain m:  82% 16%



- Molecule 37: 60S ribosomal protein L6-B

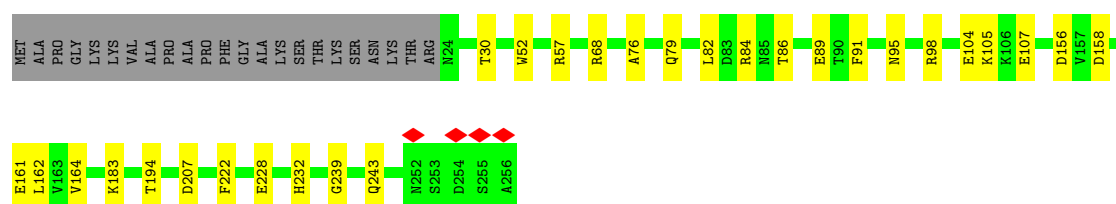
Chain n:  89% 6% 5%



- Molecule 38: 60S ribosomal protein L7-A

MET	ALA	ALA	GLU	ILE	LEU	THR	PRO	GLU	SER	GLN	LEU	LYS	LYS	SER	LYS	ALA	GLN	GLN	LYS	THR	A23	R30	R41	K70	L83	V86	V87	K94	G114	T115	F116	K121	R232	F235	M243	V244
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------

Chain p: 80% 11% 9%



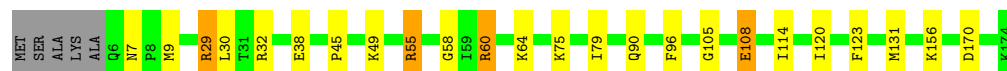
Chain q: 87% 12%



Chain r: 87% 11%



Chain s: 83% 11% 6%



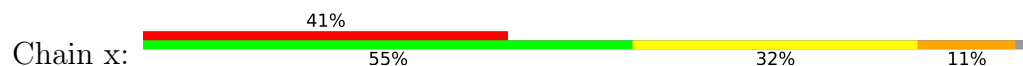
Chain t: 88% 9%

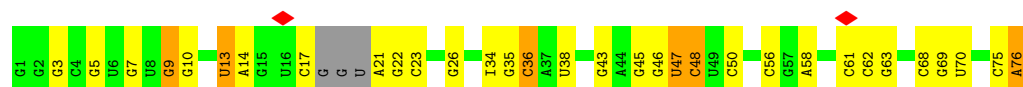


Chain u: 88% 11%

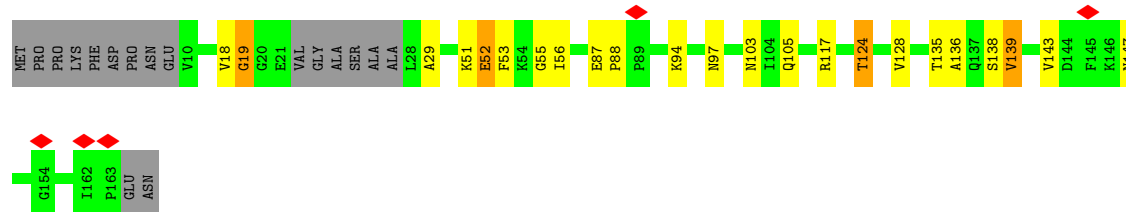




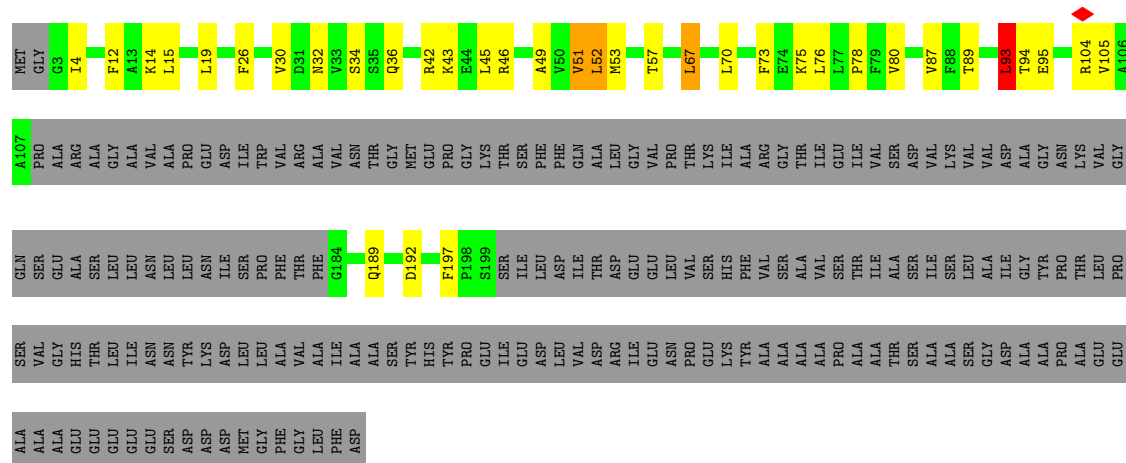




Chain z: 76% 12% 10%



Chain 0: 27% 10% 61%



Chain 1: 56% 44%

X41	X42	X43	X44	X45	X46	X56	X57	X58
-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	124605	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 ($e^-/\text{\AA}^2$)	46	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.973	Depositor
Minimum map value	-0.648	Depositor
Average map value	0.020	Depositor
Map value standard deviation	0.132	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	476.55002, 476.55002, 476.55002	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, SPD, 5CT

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	A	0.31	0/1757	0.54	0/2354
2	B	0.32	0/1585	0.54	0/2128
3	C	0.41	1/1439 (0.1%)	0.71	2/1938 (0.1%)
4	D	0.28	0/1465	0.57	0/1965
5	E	0.33	0/1275	0.61	1/1702 (0.1%)
6	F	0.31	0/1473	0.56	0/1980
7	G	0.27	0/1296	0.56	0/1739
8	H	0.47	0/828	0.86	5/1121 (0.4%)
9	I	0.27	0/1018	0.50	0/1369
10	J	0.27	0/530	0.52	0/703
11	K	0.31	0/979	0.57	0/1321
12	L	0.27	0/995	0.53	0/1329
13	M	0.27	0/1106	0.56	0/1485
14	N	0.32	0/1200	0.56	1/1607 (0.1%)
15	O	0.25	0/473	0.62	0/629
16	P	0.26	0/745	0.60	0/1001
17	Q	0.44	0/890	0.67	0/1196
18	R	0.26	0/1034	0.47	0/1385
19	S	0.30	0/868	0.47	0/1168
20	T	0.29	0/890	0.58	2/1189 (0.2%)
21	U	0.27	0/978	0.53	0/1301
22	V	0.28	0/772	0.57	0/1026
23	W	0.32	0/660	0.60	0/875
24	X	0.29	0/618	0.65	1/826 (0.1%)
25	Y	0.29	0/443	0.46	0/588
26	Z	0.28	0/416	0.60	0/553
27	b	0.28	0/836	0.53	0/1104
28	c	0.27	0/701	0.56	0/934
29	d	0.22	0/208	0.81	2/267 (0.7%)
30	f	0.30	0/76989	0.39	5/120031 (0.0%)
31	h	0.26	0/2883	0.32	0/4491
32	i	0.30	0/3746	0.36	0/5832

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	j	0.31	0/1908	0.54	0/2564
34	k	0.29	0/3146	0.53	0/4228
35	l	0.29	0/2800	0.57	4/3790 (0.1%)
36	m	0.27	0/2400	0.56	0/3239
37	n	0.28	0/1329	0.60	0/1794
38	o	0.31	0/1821	0.58	0/2451
39	p	0.27	0/1836	0.58	1/2481 (0.0%)
40	q	0.30	0/1529	0.63	2/2060 (0.1%)
41	r	0.25	0/1801	0.49	0/2416
42	s	0.34	0/1367	0.73	4/1834 (0.2%)
43	t	0.29	0/1568	0.62	1/2106 (0.0%)
44	u	0.30	0/1068	0.53	0/1438
45	a	0.27	0/6689	0.56	2/9023 (0.0%)
46	e	0.70	0/11707	1.05	81/15897 (0.5%)
47	v	0.25	0/1084	0.61	1/1456 (0.1%)
48	w	0.29	0/1736	0.62	1/2332 (0.0%)
49	x	0.26	0/1760	0.41	0/2738
49	y	0.31	1/1734 (0.1%)	0.44	0/2697
50	z	0.67	0/726	1.26	14/1006 (1.4%)
51	0	0.49	0/976	0.95	3/1313 (0.2%)
All	All	0.35	2/160081 (0.0%)	0.54	133/234000 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1
5	E	0	1
8	H	0	1
15	O	0	1
21	U	0	1
34	k	0	1
35	l	0	2
39	p	0	3
40	q	0	1
44	u	0	1
46	e	0	1
All	All	0	14

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	y	34	I	O3'-P	7.13	1.63	1.56
3	C	129	THR	CA-C	-6.80	1.44	1.52

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	e	1364	GLY	N-CA-C	11.33	126.20	112.49
46	e	1460	SER	N-CA-C	11.12	123.48	111.36
46	e	1004	ASN	N-CA-C	11.05	123.40	111.36
46	e	553	GLN	N-CA-C	-10.44	93.58	109.14
46	e	1524	SER	N-CA-C	9.37	121.26	111.14
46	e	1447	LYS	N-CA-C	-9.36	98.17	110.53
46	e	1298	GLY	N-CA-C	-9.27	100.80	115.08
46	e	204	SER	N-CA-C	-9.03	101.44	111.28
3	C	129	THR	CA-C-N	-9.02	110.12	122.30
3	C	129	THR	C-N-CA	-9.02	110.12	122.30
46	e	934	ALA	N-CA-C	-8.79	101.70	111.28
46	e	57	ARG	N-CA-C	8.72	120.79	111.28
46	e	994	ASP	N-CA-C	8.65	120.33	111.07
46	e	571	LYS	N-CA-C	8.44	120.48	111.28
46	e	896	PHE	N-CA-C	7.89	119.97	111.36
8	H	51	GLY	CA-C-N	7.86	136.56	121.54
8	H	51	GLY	C-N-CA	7.86	136.56	121.54
46	e	205	GLU	N-CA-C	-7.85	102.72	111.28
45	a	116	PHE	N-CA-C	-7.73	103.91	112.72
46	e	1002	LEU	N-CA-C	-7.72	102.87	111.28
46	e	796	LEU	N-CA-C	-7.69	102.97	111.36
46	e	885	GLN	N-CA-C	-7.67	94.88	108.69
46	e	1181	ASP	N-CA-C	7.65	119.69	111.36
47	v	53	GLY	N-CA-C	7.63	124.19	112.51
46	e	993	VAL	N-CA-C	7.53	118.32	110.72
46	e	1182	LYS	N-CA-C	7.37	118.96	111.07
50	z	87	GLU	CA-C-N	-7.36	112.80	120.38
50	z	87	GLU	C-N-CA	-7.36	112.80	120.38
46	e	148	SER	N-CA-C	7.26	118.98	111.14
50	z	138	SER	N-CA-C	-7.23	103.33	111.14
45	a	117	PHE	N-CA-CB	-7.03	100.31	110.36
46	e	79	ASN	N-CA-C	7.02	121.44	113.01
46	e	1449	TYR	CA-C-N	-6.97	111.32	119.05
46	e	1449	TYR	C-N-CA	-6.97	111.32	119.05
46	e	306	VAL	N-CA-C	6.93	117.72	110.72
46	e	1340	TYR	N-CA-C	-6.92	98.54	109.07
46	e	798	LEU	N-CA-C	6.90	118.80	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	93	ILE	N-CA-C	6.81	117.92	107.78
50	z	94	LYS	N-CA-C	-6.80	103.95	111.36
46	e	1076	SER	N-CA-C	-6.79	103.96	111.36
35	l	4	PRO	CA-C-N	6.76	134.45	121.54
35	l	4	PRO	C-N-CA	6.76	134.45	121.54
46	e	1551	CYS	CA-C-N	-6.72	111.44	119.84
46	e	1551	CYS	C-N-CA	-6.72	111.44	119.84
46	e	1557	GLU	N-CA-C	6.70	119.94	110.50
46	e	1483	MET	N-CA-C	-6.66	100.35	110.14
46	e	1069	GLY	N-CA-C	6.60	123.02	111.14
46	e	577	THR	N-CA-C	-6.50	104.23	111.71
46	e	1240	LEU	CA-C-N	-6.43	112.88	119.83
46	e	1240	LEU	C-N-CA	-6.43	112.88	119.83
46	e	773	PHE	N-CA-C	6.42	118.08	111.14
14	N	66	ALA	N-CA-C	-6.38	106.46	114.56
46	e	893	MET	N-CA-C	-6.34	104.37	111.28
46	e	258	THR	N-CA-C	-6.31	105.54	113.18
40	q	138	THR	CA-C-N	6.28	133.54	121.54
40	q	138	THR	C-N-CA	6.28	133.54	121.54
46	e	737	TYR	N-CA-C	6.27	120.56	112.41
46	e	635	LYS	N-CA-C	-6.26	104.95	112.59
46	e	897	ASP	N-CA-C	6.26	118.10	111.28
46	e	965	ASN	N-CA-C	-6.23	104.55	111.71
29	d	4	MET	CA-C-N	6.20	133.38	121.54
29	d	4	MET	C-N-CA	6.20	133.38	121.54
46	e	1064	GLY	N-CA-C	6.20	120.17	112.73
46	e	1535	HIS	N-CA-C	-6.01	102.03	110.50
46	e	733	HIS	N-CA-C	-5.89	104.86	111.28
50	z	124	THR	N-CA-C	5.86	117.66	111.28
46	e	1338	SER	CA-C-N	-5.83	112.56	119.84
46	e	1338	SER	C-N-CA	-5.83	112.56	119.84
46	e	770	ILE	CB-CA-C	-5.80	104.31	112.14
46	e	1054	ASP	N-CA-C	5.78	117.25	111.07
46	e	1518	VAL	N-CA-C	5.75	116.52	110.72
5	E	33	ALA	N-CA-C	-5.73	106.29	113.28
46	e	275	GLY	N-CA-C	-5.72	107.42	115.32
46	e	1391	ILE	N-CA-C	5.72	116.50	110.72
30	f	2541	U	P-O3'-C3'	5.68	128.72	120.20
46	e	971	ASP	N-CA-C	5.67	117.46	111.28
46	e	437	LYS	CB-CA-C	-5.63	110.09	116.63
42	s	114	ILE	CA-C-N	5.63	132.29	121.54
42	s	114	ILE	C-N-CA	5.63	132.29	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	s	7	ASN	N-CA-C	5.58	117.61	109.30
46	e	1163	GLU	N-CA-C	5.53	118.24	110.23
46	e	1255	GLU	N-CA-C	5.51	117.64	110.53
46	e	1090	ASP	N-CA-C	5.50	117.28	111.28
20	T	94	LEU	CA-C-N	-5.48	112.69	121.35
20	T	94	LEU	C-N-CA	-5.48	112.69	121.35
46	e	30	PHE	N-CA-C	5.47	117.25	111.28
43	t	136	GLU	CA-CB-CG	5.46	125.03	114.10
46	e	1551	CYS	N-CA-C	-5.46	101.62	109.48
50	z	52	GLU	N-CA-C	-5.46	104.76	111.75
46	e	697	LEU	N-CA-C	-5.45	101.99	110.10
46	e	1549	ASN	N-CA-C	5.42	118.91	111.54
50	z	19	GLY	N-CA-C	5.41	119.46	112.54
42	s	108	GLU	CA-CB-CG	5.39	124.88	114.10
46	e	989	GLU	N-CA-C	-5.38	105.42	111.28
46	e	5	GLY	N-CA-C	5.36	118.30	112.29
46	e	793	ASN	N-CA-C	-5.36	105.54	111.71
46	e	593	PHE	N-CA-C	-5.36	102.95	110.50
46	e	652	GLN	N-CA-C	-5.36	105.44	111.28
51	0	94	THR	N-CA-C	5.35	117.11	111.28
30	f	1307	G	P-O3'-C3'	5.35	128.22	120.20
30	f	2502	A	P-O3'-C3'	5.34	128.22	120.20
46	e	1252	VAL	CA-C-N	-5.34	113.66	120.23
46	e	1252	VAL	C-N-CA	-5.34	113.66	120.23
30	f	282	G	C2'-C3'-O3'	5.33	121.69	113.70
46	e	16	LEU	N-CA-C	-5.33	106.56	113.16
8	H	103	TYR	N-CA-C	5.32	116.95	110.41
30	f	1815	U	P-O3'-C3'	5.31	128.17	120.20
46	e	548	ILE	CB-CA-C	-5.30	108.74	114.35
50	z	117	ARG	N-CA-C	-5.28	105.53	111.28
50	z	29	ALA	N-CA-C	-5.27	105.67	113.16
46	e	1250	ASP	N-CA-C	5.26	117.09	111.36
46	e	1124	GLY	N-CA-C	5.24	125.60	113.18
8	H	91	ASP	N-CA-CB	5.21	119.30	110.49
39	p	79	GLN	CA-CB-CG	5.20	124.50	114.10
35	l	317	PRO	CA-C-N	5.19	131.46	121.54
35	l	317	PRO	C-N-CA	5.19	131.46	121.54
46	e	1375	LYS	N-CA-C	5.18	116.93	111.28
51	0	89	THR	N-CA-C	5.18	117.86	109.06
50	z	18	VAL	N-CA-C	-5.16	102.92	109.58
46	e	819	LEU	N-CA-C	-5.15	105.66	111.28
50	z	147	ASN	CA-C-N	-5.14	114.28	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	z	147	ASN	C-N-CA	-5.14	114.28	119.83
46	e	1461	ARG	N-CA-C	5.14	118.48	111.39
46	e	1480	ILE	N-CA-C	5.14	115.91	110.72
46	e	1062	PHE	N-CA-C	-5.12	102.47	110.10
46	e	1439	LEU	N-CA-C	-5.12	100.18	108.52
50	z	103	ASN	N-CA-C	5.10	116.94	109.24
24	X	67	GLN	N-CA-CB	5.09	118.70	110.40
51	0	104	ARG	N-CA-C	5.09	118.46	111.54
46	e	851	LEU	N-CA-C	5.08	116.89	111.36
46	e	1509	ALA	N-CA-C	5.06	116.79	111.28
50	z	139	VAL	N-CA-C	5.03	115.26	110.53
48	w	15	GLU	N-CA-CB	5.03	118.07	110.28

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	126	ARG	Mainchain
5	E	32	ILE	Mainchain
8	H	90	ARG	Mainchain
15	O	20	GLY	Peptide
21	U	83	LYS	Peptide
46	e	392	GLY	Peptide
34	k	141	GLY	Peptide
35	l	13	GLY	Peptide
35	l	318	LEU	Peptide
39	p	158	ASP	Peptide
39	p	30	THR	Peptide
39	p	76	ALA	Peptide
40	q	21	LYS	Peptide
44	u	12	TRP	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	A	1720	0	1779	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1555	0	1659	18	0
3	C	1416	0	1433	18	0
4	D	1441	0	1543	15	0
5	E	1258	0	1342	15	0
6	F	1437	0	1475	19	0
7	G	1272	0	1312	14	0
8	H	812	0	829	11	0
9	I	1003	0	1048	8	0
10	J	518	0	542	6	0
11	K	964	0	1025	1	0
12	L	984	0	1075	7	0
13	M	1080	0	1122	7	0
14	N	1169	0	1211	14	0
15	O	462	0	491	8	0
16	P	737	0	792	4	0
17	Q	876	0	912	6	0
18	R	1013	0	1077	8	0
19	S	850	0	880	4	0
20	T	880	0	942	8	0
21	U	969	0	1078	5	0
22	V	766	0	844	7	0
23	W	645	0	645	12	0
24	X	612	0	682	6	0
25	Y	436	0	475	2	0
26	Z	410	0	442	5	0
27	b	824	0	888	13	0
28	c	694	0	734	8	0
29	d	207	0	250	3	0
30	f	68782	0	34563	333	0
31	h	2579	0	1304	9	0
32	i	3353	0	1695	13	0
33	j	1874	0	1943	25	0
34	k	3075	0	3142	20	0
35	l	2748	0	2859	24	0
36	m	2351	0	2294	31	0
37	n	1307	0	1377	7	0
38	o	1784	0	1862	9	0
39	p	1804	0	1877	16	0
40	q	1508	0	1572	16	0
41	r	1764	0	1804	17	0
42	s	1346	0	1370	17	0
43	t	1543	0	1608	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	u	1053	0	1149	11	0
45	a	6579	0	6482	71	0
46	e	11508	0	10764	289	0
47	v	1085	0	1087	17	0
48	w	1709	0	1799	22	0
49	x	1579	0	798	14	0
49	y	1556	0	788	16	0
50	z	728	0	337	18	0
51	0	961	0	979	45	0
52	1	90	0	22	8	0
53	A	1	0	0	0	0
53	C	1	0	0	0	0
53	E	1	0	0	0	0
53	I	1	0	0	0	0
53	R	1	0	0	0	0
53	T	1	0	0	0	0
53	f	3	0	0	0	0
53	h	1	0	0	0	0
53	j	2	0	0	0	0
53	k	1	0	0	0	0
54	T	1	0	0	0	0
54	W	1	0	0	0	0
54	Z	1	0	0	0	0
54	b	1	0	0	0	0
54	c	1	0	0	0	0
54	e	2	0	0	0	0
55	f	10	0	19	1	0
All	All	149706	0	112021	1080	0

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

All (1080) 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)
46:e:271:LEU:HD13	46:e:277:MET:SD	1.52	1.50
30:f:1259:A:C8	51:0:53:MET:HB2	1.51	1.45
30:f:1258:U:H4'	51:0:42:ARG:NH1	1.26	1.40
30:f:1258:U:C4'	51:0:42:ARG:HH12	1.36	1.35
46:e:271:LEU:CD1	46:e:277:MET:SD	2.14	1.33
30:f:1257:C:H5'	50:z:124:THR:CB	1.74	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:f:1259:A:C8	51:0:53:MET:CB	2.32	1.11
46:e:203:GLU:HA	46:e:206:PHE:CB	1.80	1.10
30:f:1221:A:C2	51:0:12:PHE:HE2	1.69	1.08
46:e:271:LEU:CB	46:e:277:MET:SD	2.41	1.08
46:e:203:GLU:O	46:e:207:ARG:N	1.86	1.07
46:e:203:GLU:CA	46:e:206:PHE:HB3	1.83	1.07
46:e:203:GLU:HA	46:e:206:PHE:HB3	1.08	1.06
46:e:271:LEU:HB3	46:e:277:MET:HG3	1.38	1.05
30:f:3338:C:H5'	46:e:1377:ARG:NH2	1.71	1.03
46:e:26:SER:OG	46:e:32:GLY:HA3	1.55	1.03
46:e:271:LEU:HB3	46:e:277:MET:CG	1.88	1.01
30:f:1259:A:N7	51:0:53:MET:CB	2.25	0.99
45:a:893:LYS:HZ3	47:v:129:ASP:HB3	1.25	0.98
30:f:3338:C:H5'	46:e:1377:ARG:HH21	1.25	0.98
30:f:1259:A:H8	51:0:53:MET:HB2	1.29	0.97
46:e:406:TRP:HB2	46:e:448:THR:CB	1.94	0.97
27:b:103:ALA:HB1	42:s:60:ARG:NH1	1.80	0.96
46:e:271:LEU:HB3	46:e:277:MET:SD	2.04	0.96
30:f:1258:U:P	51:0:46:ARG:HH22	1.89	0.95
50:z:19:GLY:HA3	50:z:55:GLY:HA2	1.48	0.94
49:y:3:G:H1	49:y:70:U:H3	1.00	0.94
49:x:3:G:H1	49:x:70:U:H3	1.17	0.93
30:f:1257:C:O3'	51:0:46:ARG:NH2	2.02	0.93
42:s:29:ARG:NH2	42:s:123:PHE:CE1	2.37	0.92
46:e:406:TRP:CB	46:e:448:THR:CB	2.47	0.92
45:a:893:LYS:NZ	47:v:129:ASP:HB3	1.84	0.91
15:O:16:ALA:O	15:O:20:GLY:HA3	1.69	0.90
30:f:1222:G:OP2	51:0:57:THR:OG1	1.90	0.89
30:f:1258:U:O5'	51:0:42:ARG:NH1	2.04	0.89
49:y:76:A:O3'	52:1:57:UNK:O	1.90	0.88
27:b:103:ALA:HB1	42:s:60:ARG:HH12	1.34	0.87
30:f:1258:U:C5'	51:0:42:ARG:HH12	1.86	0.87
42:s:29:ARG:NH2	42:s:123:PHE:HE1	1.74	0.85
45:a:32:ILE:HG13	45:a:38:GLN:HB3	1.59	0.84
30:f:1221:A:C2	51:0:12:PHE:CE2	2.62	0.84
30:f:1259:A:N7	51:0:53:MET:HG3	1.92	0.83
46:e:130:LYS:HA	46:e:173:PHE:CE1	2.13	0.83
30:f:1258:U:H4'	51:0:42:ARG:HH12	0.66	0.83
30:f:1229:G:H4'	51:0:32:ASN:OD1	1.80	0.81
46:e:314:LEU:HD23	46:e:361:LEU:HD22	1.61	0.81
30:f:1222:G:N7	51:0:57:THR:HB	1.95	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:e:968:ASN:HA	46:e:973:ILE:HG13	1.64	0.80
46:e:271:LEU:HB2	46:e:277:MET:SD	2.22	0.80
46:e:884:ILE:HG21	46:e:935:SER:HB3	1.63	0.79
46:e:271:LEU:HD12	46:e:277:MET:SD	2.23	0.79
46:e:796:LEU:HD22	46:e:797:LEU:HD23	1.64	0.79
8:H:88:GLN:HE22	46:e:1372:LEU:HD11	1.47	0.78
46:e:26:SER:OG	46:e:32:GLY:CA	2.28	0.78
46:e:271:LEU:CG	46:e:277:MET:SD	2.71	0.78
30:f:1258:U:C5'	51:0:42:ARG:NH1	2.46	0.77
30:f:1259:A:N7	51:0:53:MET:CG	2.47	0.77
30:f:3337:G:O2'	46:e:1377:ARG:NH2	2.20	0.74
30:f:1258:U:C4'	51:0:42:ARG:NH1	2.13	0.74
15:O:16:ALA:O	15:O:20:GLY:CA	2.36	0.73
45:a:671:SER:O	48:w:98:LYS:HE2	1.88	0.73
45:a:426:GLU:HG3	46:e:9:PHE:HB3	1.69	0.73
50:z:105:GLN:HA	50:z:143:VAL:HA	1.71	0.73
46:e:372:ASP:HB3	46:e:375:LEU:HB2	1.72	0.72
5:E:31:GLU:HA	5:E:34:GLN:HB2	1.71	0.71
46:e:1187:ASN:HB3	46:e:1190:GLN:HG2	1.72	0.71
40:q:92:TYR:HB2	40:q:142:ASP:HB3	1.73	0.70
30:f:1018:G:H1	30:f:1034:U:H3	1.38	0.69
30:f:1219:C:OP1	51:0:4:ILE:HG21	1.92	0.69
46:e:1189:ASN:HD21	46:e:1337:PHE:HB3	1.58	0.69
23:W:21:ARG:HE	23:W:39:TYR:HB2	1.58	0.69
51:0:26:PHE:HB2	51:0:87:VAL:HB	1.73	0.69
46:e:987:ILE:HD11	46:e:996:GLU:HG3	1.74	0.69
46:e:930:ASN:HA	46:e:933:LEU:HB2	1.73	0.68
30:f:2193:U:H5'	30:f:2194:G:H5'	1.75	0.68
2:B:46[A]:GLU:HB3	2:B:49[A]:ARG:HG3	1.75	0.68
30:f:1222:G:C8	51:0:57:THR:HB	2.29	0.68
48:w:138:VAL:HG23	48:w:147:LYS:HD2	1.75	0.67
45:a:90:THR:HG21	45:a:107:ASP:OD1	1.94	0.67
46:e:889:GLY:HA2	46:e:897:ASP:HB2	1.77	0.67
46:e:796:LEU:HD22	46:e:797:LEU:CD2	2.24	0.67
46:e:937:GLU:HB2	46:e:972:GLU:HB3	1.76	0.67
42:s:29:ARG:HH22	42:s:123:PHE:HE1	1.44	0.66
46:e:436:GLY:HA2	46:e:482:ASN:CB	2.25	0.66
49:y:76:A:O3'	52:1:58:UNK:C	2.43	0.66
30:f:1222:G:C8	51:0:57:THR:CB	2.79	0.66
30:f:1764:U:H3'	30:f:1765:U:H4'	1.75	0.66
46:e:777:MET:HG2	46:e:904:VAL:HG11	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:f:1240:A:OP1	50:z:97:ASN:O	2.14	0.66
30:f:1254:C:O2	50:z:135:THR:CB	2.43	0.66
30:f:1222:G:C8	51:0:57:THR:HG21	2.31	0.66
46:e:203:GLU:C	46:e:206:PHE:HB3	2.21	0.66
46:e:1053:LEU:HG	46:e:1079:LEU:HD12	1.76	0.66
30:f:1940:G:H21	30:f:3362:A:H8	1.44	0.66
46:e:1213:TYR:HA	46:e:1238:PHE:CZ	2.31	0.66
30:f:1258:U:P	51:0:46:ARG:NH2	2.64	0.66
30:f:1221:A:N3	51:0:12:PHE:HE2	1.94	0.65
30:f:1238:C:H4'	50:z:139:VAL:CB	2.27	0.65
30:f:2969:A:N7	33:j:215:ASN:ND2	2.43	0.65
46:e:1374:ILE:HB	46:e:1380:GLN:HG3	1.77	0.65
46:e:876:PHE:HB3	46:e:924:VAL:HB	1.79	0.65
23:W:2:GLY:N	30:f:2138:A:HO2'	1.94	0.65
30:f:687:U:OP2	43:t:36:ARG:NH2	2.30	0.65
46:e:865:THR:HB	46:e:868:LYS:HB2	1.79	0.65
46:e:406:TRP:HB3	46:e:448:THR:CB	2.27	0.65
7:G:84:TYR:HB2	15:O:24:PRO:HD3	1.78	0.64
46:e:1210:ILE:O	46:e:1214:GLU:HG3	1.97	0.64
30:f:3338:C:C5'	46:e:1377:ARG:NH2	2.54	0.64
5:E:128:LYS:NZ	30:f:1724:U:OP2	2.31	0.64
45:a:672:ASP:HA	48:w:98:LYS:HE3	1.80	0.64
46:e:1086:MET:HB3	46:e:1098:LEU:HD13	1.80	0.63
45:a:431:ASN:HD21	46:e:12:TYR:HD2	1.45	0.63
2:B:27[A]:LEU:HD21	2:B:102[A]:LEU:HB2	1.80	0.63
46:e:795:HIS:HB3	46:e:1047:THR:HB	1.79	0.63
9:I:12:ARG:NH1	30:f:3041:U:OP1	2.32	0.63
46:e:1165:LYS:HA	46:e:1168:GLU:CD	2.23	0.62
30:f:2442:G:H1	30:f:2505:U:H3	1.46	0.62
46:e:1050:LEU:HD21	46:e:1098:LEU:HD23	1.81	0.62
28:c:87:ARG:NH1	33:j:97:ASN:OD1	2.33	0.62
45:a:403:LYS:NZ	45:a:512:LEU:O	2.28	0.62
46:e:16:LEU:HD22	46:e:22:GLY:HA2	1.80	0.62
13:M:27:LYS:HB3	13:M:42:LEU:HB2	1.81	0.62
29:d:4:MET:N	30:f:1802:C:OP1	2.32	0.62
30:f:1232:C:O2'	51:0:36:GLN:NE2	2.31	0.62
46:e:203:GLU:O	46:e:206:PHE:HB3	2.00	0.62
46:e:1382:ASP:HA	46:e:1385:LYS:HE2	1.81	0.62
9:I:14:SER:O	9:I:81:GLN:NE2	2.33	0.62
5:E:31:GLU:C	5:E:34:GLN:H	2.08	0.62
46:e:241:LEU:HB3	46:e:283:ILE:HG21	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:21:ARG:HG2	32:i:103:G:H4'	1.82	0.61
30:f:1221:A:N3	51:0:12:PHE:CE2	2.67	0.61
46:e:972:GLU:HA	46:e:975:LYS:HD2	1.80	0.61
46:e:1035:LEU:HA	46:e:1040:ALA:HB2	1.82	0.61
30:f:1348:U:O2	30:f:1349:G:N2	2.34	0.61
36:m:50:ARG:NH1	36:m:147:ASP:OD2	2.34	0.61
38:o:87:VAL:HG11	38:o:243:MET:HE1	1.83	0.61
30:f:3348:G:H1	30:f:3357:U:H3	1.48	0.61
30:f:1235:U:O4	50:z:136:ALA:HA	2.00	0.61
36:m:294:ALA:HB1	41:r:217:PHE:HB3	1.83	0.61
46:e:203:GLU:O	46:e:206:PHE:N	2.34	0.61
46:e:1303:MET:HE2	46:e:1303:MET:HA	1.83	0.60
46:e:697:LEU:O	46:e:698:TYR:HB2	2.00	0.60
46:e:1099:ARG:HG2	46:e:1100:SER:N	2.16	0.60
4:D:38:ARG:NH2	30:f:1348:U:OP2	2.34	0.60
20:T:74:ARG:NH2	30:f:1639:C:OP2	2.31	0.60
3:C:173:ARG:NH2	30:f:618:C:OP1	2.35	0.60
8:H:27:VAL:HG21	8:H:107:PHE:CE1	2.37	0.60
46:e:750:ALA:HB1	46:e:822:LEU:HD11	1.83	0.60
6:F:80:ARG:HH21	6:F:87:THR:HG21	1.66	0.60
14:N:21:ARG:NH2	30:f:640:U:OP1	2.32	0.60
40:q:89:LYS:HG2	40:q:145:VAL:HG22	1.84	0.60
46:e:997:PHE:HA	46:e:1000:LEU:HD12	1.82	0.60
1:A:201:ARG:NH2	30:f:692:A:OP1	2.35	0.60
30:f:1253:U:H5''	30:f:1254:C:H5'	1.83	0.60
23:W:55:ARG:NH2	35:l:59:GLN:OE1	2.34	0.59
46:e:770:ILE:HG23	46:e:902:ASN:HB2	1.84	0.59
6:F:8:GLN:HB3	6:F:64:ILE:HD11	1.84	0.59
31:h:31:U:O2'	36:m:218:ARG:NH1	2.35	0.59
43:t:27:ASP:O	43:t:31:LYS:HB2	2.01	0.59
47:v:43:ASP:HB3	47:v:60:VAL:HB	1.83	0.59
36:m:277:LEU:HG	36:m:281:GLU:HG3	1.82	0.59
51:0:192:ASP:HB2	51:0:197:PHE:HE2	1.67	0.59
1:A:183:THR:HG22	1:A:187:ARG:HB2	1.85	0.59
45:a:4:ARG:NH1	45:a:57:GLY:O	2.35	0.59
45:a:975:LYS:HE2	45:a:998:LYS:HA	1.84	0.59
46:e:1077:GLU:HB2	46:e:1123:TYR:H	1.67	0.59
52:1:44:UNK:O	52:1:46:UNK:N	2.36	0.59
31:h:52:G:H21	42:s:9:MET:HE1	1.68	0.59
33:j:27:ALA:O	33:j:128:ARG:NH2	2.36	0.59
21:U:5:LYS:HB2	21:U:8:GLU:HG2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:f:439:C:O2'	30:f:494:G:N2	2.34	0.59
30:f:1268:G:O2'	30:f:1273:A:N6	2.36	0.59
30:f:804:C:OP1	35:l:98:ARG:NH2	2.35	0.58
46:e:770:ILE:HG13	46:e:898:ILE:HG23	1.86	0.58
14:N:21:ARG:NH1	30:f:1369:A:OP1	2.36	0.58
28:c:4:ARG:NH1	30:f:837:A:OP2	2.37	0.58
45:a:619:HIS:NE2	45:a:679:GLY:O	2.36	0.58
48:w:65:ILE:HG12	48:w:109:ALA:HB3	1.85	0.58
30:f:2854:U:OP2	41:r:3:ARG:NH2	2.37	0.58
5:E:100:ARG:NH1	30:f:1722:U:OP1	2.36	0.58
30:f:1354:G:N3	37:n:8:LYS:NZ	2.51	0.58
6:F:77:VAL:HG22	6:F:126:VAL:HG23	1.85	0.58
14:N:42:ARG:NH2	30:f:2800:G:O6	2.37	0.58
28:c:17:ARG:NH1	30:f:860:G:OP1	2.36	0.58
41:r:205:SER:OG	41:r:208:ASN:OD1	2.21	0.58
30:f:1259:A:N7	51:0:53:MET:HB3	2.15	0.58
32:i:21:C:OP1	35:l:193:LYS:NZ	2.36	0.58
46:e:1407:MET:HG3	46:e:1419:ILE:HD12	1.86	0.58
51:0:43:LYS:HA	51:0:46:ARG:HG2	1.86	0.58
30:f:3187:A:OP1	40:q:23:ARG:NH1	2.37	0.57
2:B:60[A]:LYS:HE3	30:f:1307:G:H5'	1.86	0.57
11:K:50:ALA:HB1	21:U:66:VAL:HG11	1.86	0.57
36:m:166:ALA:HB1	36:m:171:LEU:HD12	1.86	0.57
45:a:32:ILE:CG1	45:a:38:GLN:HB3	2.34	0.57
45:a:359:GLN:HA	45:a:362:LYS:HD2	1.86	0.57
46:e:952:LYS:H	46:e:952:LYS:HD2	1.68	0.57
45:a:936:ASP:HA	45:a:996:MET:HE1	1.86	0.57
46:e:1210:ILE:HG12	46:e:1286:MET:HE1	1.85	0.57
26:Z:125:LYS:O	40:q:173:ARG:NH1	2.35	0.57
36:m:64:ILE:HG13	36:m:109:THR:HG21	1.87	0.57
45:a:151:MET:HE3	49:x:36:C:H42	1.69	0.57
28:c:4:ARG:NH2	30:f:838:G:O6	2.38	0.57
30:f:2842:U:OP1	30:f:2844:C:N4	2.37	0.57
46:e:1467:GLN:HG3	46:e:1468:LYS:N	2.20	0.57
50:z:51:LYS:O	50:z:55:GLY:N	2.38	0.57
30:f:1390:A:N6	30:f:1418:A:O2'	2.38	0.56
34:k:59:ASP:HB2	34:k:357:LYS:HE3	1.87	0.56
49:y:13:U:H2'	49:y:14:A:H8	1.70	0.56
52:1:44:UNK:C	52:1:46:UNK:N	2.67	0.56
46:e:203:GLU:O	46:e:206:PHE:CA	2.53	0.56
46:e:831:ASN:HB2	46:e:834:ILE:HG13	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:43:PRO:HB2	30:f:728:G:H5''	1.86	0.56
37:n:132:THR:HA	37:n:135:VAL:HG12	1.87	0.56
45:a:893:LYS:CE	47:v:129:ASP:HB3	2.35	0.56
13:M:17:ARG:NH1	30:f:1634:G:N7	2.53	0.56
26:Z:100:TYR:O	30:f:2895:G:O2'	2.24	0.56
30:f:1231:A:H5''	30:f:1232:C:H5'	1.86	0.56
46:e:1013:ASP:HB3	46:e:1016:PHE:HB3	1.88	0.56
3:C:129:THR:N	3:C:137:ASN:O	2.34	0.56
22:V:68:ARG:NH2	30:f:2219:A:OP2	2.38	0.56
47:v:49:THR:HG22	47:v:56:LYS:HE3	1.87	0.56
25:Y:5:LYS:HE2	25:Y:13:MET:HE1	1.87	0.56
28:c:49:ARG:NH2	30:f:1793:C:OP2	2.38	0.56
30:f:542:G:H1	30:f:549:U:H3	1.52	0.56
17:Q:55:LEU:HB2	17:Q:95:PRO:HD3	1.86	0.56
34:k:66:LYS:O	34:k:70:ARG:NH2	2.39	0.56
46:e:845:VAL:HG11	46:e:860:TYR:HA	1.88	0.56
46:e:839:THR:HB	46:e:866:PHE:H	1.71	0.56
36:m:75:LEU:O	36:m:112:LYS:NZ	2.40	0.55
41:r:143:SER:C	41:r:144:ASN:HD22	2.14	0.55
45:a:412:GLN:HG2	46:e:4:GLY:O	2.06	0.55
20:T:87:GLU:OE2	20:T:91:ARG:NH1	2.39	0.55
46:e:968:ASN:HD22	46:e:1009:ILE:HG12	1.70	0.55
8:H:93:ILE:HG21	8:H:105:LEU:HD23	1.88	0.55
46:e:79:ASN:HA	46:e:82:PHE:HB2	1.88	0.55
45:a:90:THR:HG21	45:a:107:ASP:H	1.70	0.55
18:R:19:ARG:HD3	18:R:33:ARG:HB2	1.89	0.55
30:f:2493:U:OP1	48:w:215:ARG:NH2	2.39	0.55
45:a:885:LYS:O	45:a:889:ARG:HG3	2.06	0.55
51:0:42:ARG:HG2	51:0:51:VAL:HG11	1.89	0.55
52:1:44:UNK:O	52:1:45:UNK:C	2.54	0.55
14:N:44:ASN:ND2	43:t:4:SER:O	2.40	0.55
33:j:111:THR:HB	33:j:136:ILE:HD13	1.87	0.55
46:e:281:LYS:O	46:e:285:LYS:HG3	2.07	0.55
30:f:394:G:N1	30:f:397:A:OP2	2.39	0.55
33:j:70:ARG:HD2	33:j:72:ARG:HE	1.72	0.55
30:f:3042:U:OP2	30:f:3092:C:N4	2.38	0.55
30:f:3045:G:OP1	34:k:19:ARG:NH2	2.39	0.55
46:e:320:LEU:HB3	46:e:328:ILE:HG21	1.88	0.55
2:B:157[A]:GLU:OE2	2:B:160[A]:ARG:NH2	2.40	0.55
45:a:1005:LEU:HA	45:a:1008:LEU:HD12	1.89	0.55
46:e:973:ILE:HD12	46:e:1006:LEU:HD21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:e:1077:GLU:HB3	46:e:1122:GLU:HG2	1.89	0.55
46:e:1028:PHE:HB3	46:e:1075:LEU:HD13	1.89	0.54
46:e:1070:ILE:HD12	46:e:1073:PHE:HD2	1.71	0.54
48:w:48:ARG:HG2	48:w:159:LEU:HD23	1.89	0.54
3:C:128:ARG:HA	3:C:137:ASN:O	2.07	0.54
30:f:1222:G:C8	51:0:57:THR:CG2	2.90	0.54
30:f:1352:A:H4'	30:f:1353:U:H5'	1.88	0.54
30:f:3231:U:H2'	30:f:3232:G:H8	1.73	0.54
40:q:57:VAL:HG12	40:q:68:LEU:HD22	1.88	0.54
41:r:61:SER:OG	41:r:63:GLU:OE1	2.25	0.54
46:e:355:PHE:HA	46:e:358:VAL:HG12	1.90	0.54
49:y:21:A:N6	49:y:48:C:OP2	2.40	0.54
40:q:23:ARG:HE	40:q:39:LYS:HA	1.71	0.54
46:e:203:GLU:C	46:e:206:PHE:H	2.15	0.54
46:e:1075:LEU:HG	46:e:1078:ARG:HD3	1.90	0.54
5:E:31:GLU:HA	5:E:34:GLN:CB	2.36	0.54
30:f:1256:G:O2'	50:z:124:THR:CB	2.55	0.54
30:f:2268:U:H3	30:f:2272:G:H22	1.55	0.54
46:e:41:SER:HB2	46:e:86:ILE:HG21	1.89	0.54
46:e:1248:VAL:HG12	46:e:1299:LEU:HD11	1.90	0.54
30:f:2674:A:H5''	42:s:105:GLY:HA3	1.89	0.54
36:m:236:LEU:HA	36:m:239:ILE:HG12	1.90	0.54
30:f:68:C:OP2	30:f:301:G:N2	2.40	0.54
46:e:1057:THR:HB	46:e:1108:THR:HG21	1.90	0.54
14:N:95:SER:OG	14:N:98:THR:OG1	2.25	0.54
30:f:76:G:O2'	43:t:100:ARG:NH1	2.37	0.54
7:G:17:ARG:HG2	7:G:22:HIS:HA	1.90	0.54
30:f:1221:A:C4	51:0:12:PHE:CE2	2.96	0.54
30:f:1221:A:C4	51:0:12:PHE:CZ	2.95	0.54
36:m:270:LYS:HG2	36:m:273:ARG:HE	1.73	0.54
46:e:107:ARG:HH21	46:e:147:VAL:HG21	1.73	0.54
30:f:2162:U:OP1	33:j:234:LYS:NZ	2.39	0.53
46:e:1273:HIS:HA	46:e:1276:LEU:HG	1.90	0.53
8:H:56:VAL:HG12	8:H:65:VAL:HG22	1.88	0.53
30:f:3268:A:OP1	37:n:46:ARG:NH2	2.35	0.53
34:k:140:ASP:OD1	34:k:141:GLY:N	2.36	0.53
30:f:3115:C:OP1	40:q:62:ARG:NH2	2.41	0.53
30:f:1156:C:OP2	38:o:94:LYS:NZ	2.40	0.53
10:J:44:LYS:HD2	30:f:2111:G:H1'	1.90	0.53
30:f:1242:G:H1	45:a:519:THR:HG22	1.73	0.53
30:f:1256:G:H4'	50:z:128:VAL:CB	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:f:1257:C:C5'	50:z:124:THR:CB	2.68	0.53
45:a:607:ASP:HB3	45:a:663:LYS:HB3	1.90	0.53
47:v:46:THR:HG22	47:v:57:VAL:HG22	1.90	0.53
10:J:6:ASP:OD1	10:J:32:GLN:N	2.40	0.53
23:W:52:LYS:NZ	35:l:59:GLN:O	2.39	0.53
30:f:3375:A:O2'	30:f:3378:C:OP2	2.26	0.53
34:k:284:ARG:NH1	34:k:293:ASN:O	2.42	0.53
42:s:32:ARG:HD2	42:s:120:ILE:HA	1.91	0.53
49:y:3:G:O6	49:y:70:U:O4	2.27	0.53
2:B:21[A]:SER:OG	30:f:1181:U:O4	2.27	0.53
2:B:75[A]:ALA:HB3	2:B:78[A]:ARG:HG2	1.90	0.53
30:f:2245:C:O2'	33:j:220:GLY:O	2.26	0.53
46:e:247:TRP:HZ2	46:e:283:ILE:HG23	1.73	0.53
46:e:790:LEU:HB3	46:e:793:ASN:HB2	1.91	0.53
6:F:96:ASP:OD1	6:F:97:VAL:N	2.38	0.53
36:m:120:LYS:O	36:m:248:ARG:NH2	2.42	0.53
49:x:55:U:H2'	49:x:56:C:H2'	1.91	0.53
20:T:31:ARG:NH2	30:f:1598:G:OP2	2.42	0.52
30:f:831:G:O2'	30:f:1864:A:N3	2.39	0.52
45:a:604:TYR:O	45:a:623:LYS:NZ	2.39	0.52
10:J:47:ARG:HH21	10:J:58:HIS:HB2	1.73	0.52
46:e:957:CYS:HA	46:e:960:LEU:HB2	1.90	0.52
49:y:13:U:H3	49:y:22:G:H1	1.56	0.52
2:B:61[A]:ALA:HA	2:B:70[A]:PRO:HD2	1.90	0.52
8:H:44:GLU:OE2	8:H:49:ASN:ND2	2.41	0.52
6:F:77:VAL:HG11	6:F:106:LEU:HD22	1.92	0.52
8:H:27:VAL:HG21	8:H:107:PHE:HE1	1.74	0.52
30:f:1288:U:H2'	30:f:1289:G:H8	1.74	0.52
30:f:3230:G:H4'	44:u:132:LYS:HD3	1.92	0.52
46:e:359:PHE:HB2	46:e:408:ASN:HB3	1.91	0.52
3:C:127:ARG:CZ	3:C:139:TYR:HD2	2.23	0.52
46:e:203:GLU:HA	46:e:206:PHE:HB2	1.84	0.52
7:G:158:THR:OG1	41:r:169:LYS:NZ	2.42	0.52
17:Q:102:LYS:NZ	30:f:3373:U:OP2	2.38	0.52
45:a:111:TYR:HB2	45:a:125:LEU:HB2	1.91	0.52
45:a:612:MET:HE1	45:a:642:CYS:HB2	1.92	0.52
9:I:94:TYR:OH	10:J:41:LYS:NZ	2.39	0.52
27:b:2:VAL:N	27:b:90:HIS:O	2.42	0.52
30:f:2177:G:OP2	33:j:128:ARG:NH1	2.43	0.52
46:e:738:PHE:CE2	46:e:817:LEU:HB3	2.45	0.52
46:e:849:ASN:O	46:e:855:PRO:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:e:1507:GLU:HG2	46:e:1514:ILE:HG12	1.91	0.52
3:C:118:GLN:NE2	3:C:147:GLU:OE2	2.39	0.52
24:X:44:LYS:NZ	30:f:1750:A:OP1	2.37	0.52
6:F:80:ARG:HB2	6:F:122:HIS:HB2	1.91	0.52
14:N:100:PRO:HG2	14:N:123:VAL:HG23	1.92	0.52
10:J:16:GLY:O	30:f:3050:U:O2'	2.27	0.51
45:a:618:SER:OG	45:a:646:SER:OG	2.26	0.51
46:e:156:THR:HG22	46:e:161:LYS:HA	1.92	0.51
7:G:136:ARG:HD2	7:G:139:ARG:HH12	1.74	0.51
30:f:3160:U:H3	30:f:3290:G:H1	1.59	0.51
46:e:130:LYS:HA	46:e:173:PHE:HE1	1.68	0.51
36:m:54:ARG:NH1	36:m:147:ASP:O	2.42	0.51
42:s:49:LYS:HG3	42:s:64:LYS:HD3	1.92	0.51
46:e:1217:ILE:HG22	46:e:1217:ILE:O	2.10	0.51
29:d:20:ARG:HA	29:d:23:VAL:HG12	1.92	0.51
30:f:1778:G:O2'	30:f:1780:G:OP2	2.28	0.51
27:b:75:VAL:HG23	27:b:76:LYS:HD2	1.93	0.51
30:f:1234:G:N2	50:z:135:THR:CB	2.73	0.51
30:f:2557:A:OP1	33:j:69:TYR:OH	2.24	0.51
36:m:50:ARG:NH2	36:m:72:ASP:OD2	2.43	0.51
20:T:96:GLU:OE2	30:f:2555:G:N1	2.42	0.51
27:b:41:ARG:NH1	30:f:284:A:OP2	2.40	0.51
30:f:2540:A:N3	30:f:2541:U:N3	2.59	0.51
30:f:3027:A:O2'	45:a:415:ASP:OD1	2.29	0.51
35:l:266:THR:HG23	35:l:267:VAL:HG13	1.92	0.51
19:S:70:LYS:HD2	30:f:585:A:H5''	1.91	0.51
21:U:67:ARG:NH2	32:i:97:A:OP1	2.44	0.51
30:f:123:A:OP1	39:p:105:LYS:NZ	2.37	0.51
40:q:22:SER:OG	40:q:39:LYS:NZ	2.44	0.51
39:p:207:ASP:OD1	39:p:207:ASP:N	2.44	0.51
45:a:704:LEU:HB3	45:a:938:ILE:HG13	1.91	0.51
46:e:1526:THR:HG22	46:e:1533:LYS:HG2	1.93	0.51
30:f:591:G:O2'	37:n:17:ALA:O	2.28	0.51
30:f:1256:G:O3'	50:z:124:THR:CB	2.59	0.51
30:f:1661:G:H2'	30:f:1662:G:C8	2.46	0.51
33:j:241:ARG:HD3	45:a:866:LEU:HD21	1.92	0.51
46:e:307:CYS:SG	46:e:308:PRO:HD3	2.50	0.51
30:f:544:C:H2'	30:f:547:G:H1	1.76	0.51
30:f:2489:C:O2'	48:w:210:MET:SD	2.69	0.51
35:l:156:LEU:HD12	35:l:159:ILE:HD12	1.94	0.51
36:m:206:GLN:NE2	36:m:210:GLU:OE2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:e:1004:ASN:HA	46:e:1007:LEU:HB2	1.92	0.51
32:i:29:U:H5''	43:t:27:ASP:HB3	1.92	0.50
45:a:579:TRP:HA	45:a:588:VAL:O	2.11	0.50
1:A:103:GLU:HG3	1:A:160:GLU:HB2	1.93	0.50
3:C:107:LEU:HD12	3:C:152:GLU:HG3	1.92	0.50
15:O:23:LYS:HG3	15:O:24:PRO:HD2	1.93	0.50
21:U:118:ILE:HD11	43:t:145:PHE:HE2	1.76	0.50
30:f:2828:G:OP2	41:r:7:ARG:NH2	2.44	0.50
35:l:126:ILE:O	35:l:129:THR:OG1	2.30	0.50
39:p:52:TRP:O	39:p:57:ARG:NH1	2.44	0.50
46:e:1077:GLU:HG3	46:e:1078:ARG:N	2.26	0.50
46:e:1467:GLN:HG3	46:e:1468:LYS:H	1.76	0.50
46:e:1472:TRP:HB3	46:e:1494:PHE:HE1	1.75	0.50
50:z:19:GLY:HA3	50:z:55:GLY:CA	2.32	0.50
30:f:110:G:OP2	43:t:73:ARG:NH2	2.42	0.50
30:f:2307:G:O2'	30:f:2310:U:OP2	2.28	0.50
47:v:18:THR:HG22	47:v:83:PRO:HA	1.93	0.50
14:N:26:ARG:NH1	30:f:938:C:OP2	2.44	0.50
30:f:655:C:H2'	30:f:656:A:H8	1.76	0.50
39:p:161:GLU:HA	39:p:164:VAL:HG22	1.93	0.50
46:e:285:LYS:HG2	46:e:331:TYR:CZ	2.46	0.50
3:C:65:SER:OG	30:f:1447:G:OP1	2.28	0.50
46:e:142:GLU:HB3	46:e:148:SER:HB3	1.92	0.50
46:e:823:LEU:HD22	46:e:830:VAL:HG22	1.93	0.50
46:e:894:LEU:HB3	46:e:909:TYR:CE2	2.47	0.50
46:e:1551:CYS:HB3	46:e:1554:CYS:O	2.12	0.50
48:w:50:SER:HA	48:w:157:PHE:O	2.11	0.50
5:E:62:ARG:HH22	30:f:3067:C:H3'	1.77	0.50
30:f:664:U:H2'	30:f:665:A:C8	2.47	0.50
30:f:2137:U:OP2	30:f:2142:A:N6	2.40	0.50
30:f:2897:A:H2'	30:f:2899:C:H5''	1.93	0.50
30:f:2948:C:OP1	34:k:244:ARG:NH2	2.36	0.50
30:f:3214:U:OP2	44:u:128:ARG:NH1	2.34	0.50
46:e:985:ILE:HD11	46:e:1023:ARG:HG3	1.92	0.50
46:e:1031:ILE:HA	46:e:1034:TRP:CE3	2.47	0.50
46:e:731:LEU:O	46:e:735:GLN:HG3	2.12	0.50
46:e:973:ILE:HG22	46:e:977:ARG:HE	1.76	0.50
48:w:59:PRO:HD2	48:w:153:SER:HA	1.93	0.50
31:h:44:C:H4'	36:m:152:ARG:HG3	1.93	0.50
46:e:1089:ILE:HB	46:e:1092:THR:HG23	1.94	0.50
46:e:1184:ILE:HD11	46:e:1267:LYS:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74[A]:ARG:O	2:B:142[A]:SER:OG	2.23	0.50
28:c:18:TYR:HB3	33:j:180:LEU:HD22	1.93	0.50
45:a:192:TYR:HE1	45:a:218:PRO:HD2	1.76	0.50
46:e:340:LEU:HD21	46:e:376:GLU:HG2	1.92	0.50
46:e:1456:VAL:HG23	46:e:1480:ILE:HD11	1.93	0.50
45:a:29:ILE:HD12	45:a:80:LEU:HB3	1.94	0.49
46:e:1192:ARG:HD2	46:e:1270:TRP:CH2	2.47	0.49
49:y:9:G:O2'	49:y:10:G:N7	2.42	0.49
46:e:989:GLU:HB3	46:e:1039:LEU:HG	1.94	0.49
2:B:46[A]:GLU:HG3	2:B:48[A]:PHE:H	1.77	0.49
3:C:60:PHE:HB3	3:C:64:ASN:HB3	1.93	0.49
5:E:34:GLN:HG3	46:e:1540:TYR:CZ	2.47	0.49
24:X:2:ALA:N	30:f:1613:A:OP1	2.46	0.49
32:i:156:U:OP2	39:p:84:ARG:NH2	2.45	0.49
1:A:83:LYS:NZ	30:f:36:C:OP2	2.42	0.49
30:f:348:A:N3	30:f:352:A:O2'	2.46	0.49
30:f:1019:G:H1	30:f:1033:U:H3	1.59	0.49
30:f:1569:U:H5'	30:f:1570:U:H5''	1.94	0.49
42:s:29:ARG:NH2	42:s:123:PHE:CZ	2.80	0.49
16:P:30:THR:HG23	16:P:91:SER:HB2	1.95	0.49
36:m:90:HIS:NE2	36:m:229:ASP:OD2	2.41	0.49
30:f:505:G:OP1	35:l:320:ASN:ND2	2.43	0.49
30:f:1264:G:N2	30:f:1265:U:O4	2.40	0.49
35:l:292:SER:OG	35:l:294:GLU:OE1	2.31	0.49
42:s:90:GLN:NE2	42:s:170:ASP:OD1	2.45	0.49
45:a:970:ILE:HD11	45:a:1016:VAL:HG11	1.95	0.49
46:e:1443:PHE:HB3	46:e:1454:ILE:HD11	1.95	0.49
48:w:138:VAL:HG21	48:w:144:LEU:HD23	1.94	0.49
4:D:56:LYS:NZ	30:f:674:G:O6	2.46	0.49
7:G:99:SER:HG	7:G:101:CYS:HG	1.60	0.49
18:R:104:ASN:ND2	30:f:1389:G:OP1	2.42	0.49
30:f:2185:G:O2'	30:f:2314:U:OP2	2.28	0.49
30:f:2901:G:O2'	30:f:3024:A:N1	2.44	0.49
52:1:42:UNK:O	52:1:43:UNK:C	2.60	0.49
6:F:155:ARG:HB2	6:F:172:TYR:HD1	1.77	0.49
7:G:108:ARG:O	7:G:112:ASN:HB2	2.12	0.49
16:P:9:SER:OG	16:P:10:ILE:N	2.39	0.49
27:b:7:THR:OG1	27:b:22:GLN:NE2	2.36	0.49
37:n:92:SER:OG	37:n:148:GLU:OE2	2.30	0.49
46:e:26:SER:CB	46:e:32:GLY:HA3	2.43	0.49
46:e:347:ARG:HB3	46:e:380:PHE:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:131:ALA:HB1	4:D:135:GLN:H	1.78	0.48
45:a:107:ASP:OD2	49:y:36:C:OP1	2.31	0.48
46:e:220:ILE:HG23	46:e:270:VAL:HG21	1.95	0.48
46:e:807:LYS:HA	46:e:810:GLN:HB3	1.95	0.48
46:e:1123:TYR:CE2	46:e:1126:GLU:HB2	2.48	0.48
46:e:1149:THR:HG22	46:e:1339:PRO:HD3	1.95	0.48
14:N:94:ALA:HA	14:N:121:VAL:HG23	1.95	0.48
39:p:91:PHE:O	39:p:95:ASN:ND2	2.46	0.48
46:e:328:ILE:HA	46:e:331:TYR:CD2	2.48	0.48
46:e:932:LEU:O	46:e:936:VAL:N	2.46	0.48
5:E:30:SER:O	5:E:34:GLN:HG2	2.13	0.48
15:O:3:LYS:HD3	30:f:2617:U:H3'	1.95	0.48
27:b:30:ALA:O	30:f:2767:U:O2'	2.29	0.48
46:e:992:LEU:HD11	46:e:1000:LEU:HD11	1.95	0.48
19:S:49:ILE:HD11	19:S:71:VAL:HG22	1.96	0.48
46:e:54:LEU:HD13	46:e:94:ILE:HD12	1.94	0.48
30:f:520:U:OP2	38:o:70:LYS:NZ	2.45	0.48
30:f:1814:A:H4'	30:f:1815:U:H5'	1.95	0.48
34:k:145:GLU:HA	34:k:148:LEU:HB2	1.95	0.48
46:e:203:GLU:C	46:e:206:PHE:N	2.71	0.48
42:s:38:GLU:HB2	42:s:45:PRO:HD3	1.95	0.48
4:D:102:ALA:HA	4:D:122:ILE:O	2.14	0.48
5:E:34:GLN:HG3	46:e:1540:TYR:CE2	2.49	0.48
13:M:133:LYS:HE3	13:M:135:ARG:HD3	1.96	0.48
30:f:1480:G:O2'	30:f:1871:U:O4	2.27	0.48
40:q:18:VAL:HG12	40:q:27:VAL:HG22	1.94	0.48
45:a:672:ASP:HA	48:w:98:LYS:CE	2.43	0.48
46:e:798:LEU:HD23	46:e:798:LEU:HA	1.64	0.48
30:f:1477:A:OP1	30:f:3075:G:O2'	2.31	0.48
30:f:2155:G:OP1	33:j:241:ARG:NH1	2.46	0.48
30:f:2209:U:C4	45:a:838:ARG:HD2	2.49	0.48
30:f:2568:C:O2'	30:f:2569:A:O4'	2.27	0.48
32:i:9:A:H2'	32:i:10:A:C8	2.49	0.48
6:F:93:GLU:HG3	6:F:140:VAL:HG11	1.95	0.48
30:f:1383:G:O3'	35:l:138:ARG:NH2	2.47	0.48
30:f:3198:U:O2	40:q:21:LYS:N	2.44	0.48
35:l:304:GLN:NE2	35:l:306:THR:O	2.42	0.48
45:a:402:VAL:HG22	45:a:433:ILE:HG23	1.95	0.48
46:e:203:GLU:O	46:e:206:PHE:C	2.53	0.48
46:e:738:PHE:CD2	46:e:817:LEU:HB3	2.48	0.48
3:C:62:ARG:NH1	30:f:412:G:OP1	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:16:ARG:HB2	30:f:974:G:H5'	1.95	0.48
27:b:45:ARG:NH1	30:f:283:G:OP1	2.46	0.48
30:f:1805:C:H2'	30:f:1806:A:H8	1.79	0.48
34:k:85:VAL:HG22	34:k:202:THR:HG22	1.95	0.48
34:k:219:ALA:HB2	34:k:336:VAL:HG23	1.96	0.48
40:q:47:LYS:H	44:u:7:VAL:HG21	1.78	0.48
42:s:29:ARG:O	42:s:30:LEU:C	2.57	0.48
46:e:84:ASN:H	46:e:87:PHE:HB3	1.79	0.48
13:M:23:VAL:HG12	13:M:45:GLY:HA3	1.94	0.47
30:f:1230:G:H4'	51:0:34:SER:HA	1.96	0.47
33:j:117:GLU:HG2	33:j:124:GLY:H	1.79	0.47
26:Z:124:LYS:NZ	30:f:2897:A:OP2	2.47	0.47
43:t:76:THR:HG22	43:t:78:ALA:H	1.80	0.47
46:e:1079:LEU:HD13	46:e:1079:LEU:HA	1.76	0.47
3:C:22:LEU:HD12	3:C:146:ILE:HD12	1.97	0.47
17:Q:75:ILE:HG12	17:Q:93:VAL:HG22	1.96	0.47
46:e:795:HIS:HA	46:e:799:THR:HG22	1.97	0.47
19:S:99:ARG:NH1	30:f:3275:U:O2'	2.48	0.47
30:f:411:U:H2'	30:f:412:G:H8	1.79	0.47
30:f:655:C:H2'	30:f:656:A:C8	2.49	0.47
46:e:1145:ASN:HB2	46:e:1147:VAL:HG22	1.96	0.47
47:v:48:LYS:HA	47:v:55:ALA:HA	1.96	0.47
51:0:26:PHE:HZ	51:0:93:LEU:HA	1.80	0.47
4:D:19:PRO:HB3	4:D:53:PHE:HA	1.96	0.47
5:E:30:SER:O	5:E:33:ALA:HB3	2.14	0.47
49:x:18:G:O4'	49:x:57:G:N2	2.47	0.47
7:G:116:ARG:NH2	30:f:1096:U:OP2	2.48	0.47
9:I:18:PRO:HA	9:I:51:ALA:HA	1.97	0.47
23:W:81:GLY:O	32:i:95:G:O2'	2.32	0.47
30:f:712:G:OP1	43:t:174:ARG:NH1	2.47	0.47
30:f:829:U:H3	30:f:895:A:H62	1.63	0.47
32:i:103:G:OP2	32:i:105:A:O2'	2.33	0.47
33:j:32:LEU:HD13	33:j:163:ARG:HD3	1.96	0.47
46:e:1249:THR:HG22	46:e:1299:LEU:HD13	1.95	0.47
46:e:1509:ALA:HB3	46:e:1534:PHE:CE1	2.50	0.47
5:E:21:LYS:HE3	5:E:55:VAL:HA	1.97	0.47
5:E:151:ARG:NH2	5:E:152:GLU:OE2	2.45	0.47
30:f:358:G:N2	30:f:361:A:OP2	2.42	0.47
30:f:912:G:OP2	33:j:9:ARG:NH2	2.45	0.47
32:i:126:A:O2'	32:i:129:C:N4	2.48	0.47
41:r:54:SER:HB3	41:r:135:ILE:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:r:66:GLU:OE1	41:r:69:ARG:NH2	2.47	0.47
45:a:572:TYR:HB2	45:a:575:GLU:HG3	1.95	0.47
46:e:792:THR:HG21	46:e:1004:ASN:HD22	1.79	0.47
46:e:1016:PHE:H	46:e:1064:GLY:HA3	1.80	0.47
46:e:1213:TYR:O	46:e:1217:ILE:HG12	2.15	0.47
48:w:89:ASP:O	48:w:92:LYS:HB2	2.14	0.47
49:x:62:C:H2'	49:x:63:G:C8	2.50	0.47
49:y:47:U:C4	49:y:50:C:H5''	2.49	0.47
4:D:170:ARG:HD2	14:N:57:GLY:HA3	1.97	0.47
34:k:211:GLN:NE2	34:k:283:TYR:O	2.44	0.47
36:m:163:LEU:HD11	36:m:175:HIS:HB3	1.97	0.47
39:p:228:GLU:O	39:p:232:HIS:ND1	2.43	0.47
46:e:723:ALA:HB1	46:e:760:THR:CG2	2.44	0.47
1:A:5:LYS:HE2	22:V:40:VAL:HG21	1.97	0.47
4:D:180:ARG:NH2	30:f:2790:A:OP1	2.42	0.47
14:N:115:LYS:HA	30:f:715:A:H5''	1.97	0.47
30:f:627:U:H2'	30:f:628:A:C8	2.50	0.47
45:a:893:LYS:HZ3	47:v:129:ASP:CB	2.11	0.47
46:e:1099:ARG:HG3	46:e:1151:PHE:CD1	2.50	0.47
5:E:128:LYS:NZ	30:f:1721:U:O4	2.38	0.47
30:f:1907:C:O2	34:k:240:ARG:NH2	2.45	0.47
30:f:2466:G:H5''	48:w:60:ARG:HH12	1.80	0.47
36:m:234:ASP:OD1	36:m:234:ASP:N	2.47	0.47
44:u:55:ARG:NH2	44:u:76:ALA:O	2.48	0.47
46:e:961:LEU:CB	46:e:1005:ASN:HB3	2.45	0.47
46:e:1410:LEU:HG	46:e:1417:LEU:HD11	1.97	0.47
30:f:835:G:O2'	30:f:857:G:N2	2.37	0.46
30:f:2491:A:H1'	48:w:207:LYS:HE2	1.97	0.46
44:u:38:ILE:HA	44:u:44:VAL:HG12	1.96	0.46
49:y:62:C:H2'	49:y:63:G:H8	1.80	0.46
45:a:660:CYS:SG	45:a:661:PHE:N	2.88	0.46
46:e:1184:ILE:HA	46:e:1191:SER:HB2	1.96	0.46
15:O:55:ALA:O	15:O:59:LYS:HB3	2.16	0.46
30:f:2815:G:N2	30:f:2818:U:O2	2.45	0.46
42:s:131:MET:HE3	42:s:131:MET:HB3	1.81	0.46
45:a:121:ASN:HD22	45:a:136:ARG:NH1	2.14	0.46
46:e:373:TYR:HE2	46:e:412:PHE:O	1.98	0.46
3:C:67:ILE:HD11	3:C:80:LYS:HB3	1.98	0.46
30:f:297:G:OP2	30:f:297:G:N2	2.41	0.46
46:e:961:LEU:HD22	46:e:1006:LEU:HD23	1.98	0.46
5:E:68:GLN:OE1	5:E:71:ARG:NH2	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:55:GLU:HB2	12:L:108:LYS:HB3	1.98	0.46
30:f:86:G:O2'	30:f:98:G:O6	2.32	0.46
35:l:326:ARG:O	38:o:41:ARG:NH2	2.48	0.46
41:r:54:SER:OG	41:r:130:ASP:O	2.33	0.46
46:e:322:ASP:HA	46:e:367:ARG:HH22	1.80	0.46
46:e:980:LEU:HD13	46:e:1003:LEU:HA	1.98	0.46
46:e:1532:ASN:HD22	46:e:1532:ASN:HA	1.55	0.46
49:x:17:C:H42	49:x:55:U:H1'	1.81	0.46
49:x:62:C:H2'	49:x:63:G:H8	1.80	0.46
50:z:51:LYS:O	50:z:52:GLU:C	2.57	0.46
2:B:59[A]:ARG:NH1	30:f:1307:G:OP1	2.48	0.46
8:H:90:ARG:O	8:H:91:ASP:HB2	2.16	0.46
12:L:74:TYR:HB3	12:L:77:LYS:HB2	1.98	0.46
13:M:28:PRO:O	13:M:29:HIS:ND1	2.48	0.46
36:m:119:TYR:OH	36:m:139:PRO:O	2.33	0.46
36:m:207:TYR:HA	36:m:210:GLU:HG2	1.97	0.46
44:u:48:GLY:HA3	44:u:53:VAL:HB	1.98	0.46
46:e:292:LEU:HD13	46:e:332:ASP:HB3	1.98	0.46
50:z:51:LYS:C	50:z:53:PHE:N	2.69	0.46
18:R:9:ILE:HG12	18:R:63:THR:HG23	1.97	0.46
45:a:4:ARG:NH1	45:a:118:SER:HA	2.30	0.46
46:e:1007:LEU:HD22	46:e:1007:LEU:HA	1.74	0.46
2:B:39[A]:GLU:HG2	2:B:40[A]:GLU:HG2	1.97	0.46
4:D:35:PHE:HE1	30:f:1348:U:H5'	1.80	0.46
13:M:133:LYS:NZ	30:f:1808:G:OP2	2.44	0.46
14:N:96:LYS:HB2	14:N:96:LYS:HE2	1.70	0.46
30:f:1152:G:OP2	30:f:1152:G:N2	2.44	0.46
30:f:2239:G:O2'	45:a:867:GLY:O	2.29	0.46
46:e:796:LEU:HD12	46:e:1001:ALA:HB3	1.97	0.46
18:R:60:ASN:HB3	18:R:63:THR:HB	1.97	0.46
20:T:95:ILE:HD11	30:f:2555:G:N7	2.30	0.46
30:f:696:C:OP2	35:l:119:ARG:NH2	2.49	0.46
30:f:1949:G:H1	30:f:2097:U:H3	1.63	0.46
45:a:101:LEU:HB2	45:a:116:PHE:HE2	1.80	0.46
46:e:149:LYS:HB3	46:e:150:PRO:HD3	1.98	0.46
30:f:1717:U:H2'	30:f:1718:G:C8	2.50	0.46
38:o:86:VAL:O	38:o:114:GLY:HA2	2.16	0.46
39:p:156:ASP:OD1	39:p:156:ASP:N	2.47	0.46
46:e:377:TRP:O	46:e:381:TRP:HD1	1.99	0.46
46:e:385:VAL:HG21	46:e:428:GLU:CB	2.46	0.46
46:e:850:CYS:HB3	46:e:1146:GLN:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:v:104:ASN:OD1	47:v:105:MET:N	2.49	0.46
48:w:92:LYS:HA	48:w:92:LYS:HD3	1.71	0.46
6:F:22:PRO:O	7:G:146:ASN:ND2	2.38	0.45
30:f:40:A:OP1	55:f:3401:SPD:N10	2.48	0.45
30:f:2392:C:O2'	34:k:266:ARG:NH2	2.48	0.45
1:A:62:TYR:OH	32:i:141:C:O3'	2.34	0.45
1:A:159:ARG:HB3	1:A:164:LEU:HB2	1.98	0.45
12:L:16:ARG:NH1	30:f:216:G:OP1	2.45	0.45
15:O:25:LYS:NZ	30:f:1106:G:O3'	2.44	0.45
19:S:14:LEU:HD11	19:S:31:LYS:HB2	1.98	0.45
30:f:494:G:H2'	30:f:495:G:H8	1.82	0.45
33:j:68:LYS:HE2	33:j:70:ARG:HH21	1.80	0.45
46:e:203:GLU:O	46:e:206:PHE:CB	2.63	0.45
46:e:757:CYS:HB2	46:e:760:THR:HG23	1.97	0.45
1:A:202:TYR:HB3	35:l:112:LYS:HG3	1.97	0.45
13:M:22:LYS:NZ	13:M:132:SER:O	2.47	0.45
17:Q:44:MET:O	17:Q:77:ARG:NH1	2.49	0.45
30:f:2218:G:H2'	30:f:2219:A:H8	1.80	0.45
30:f:3022:G:O2'	30:f:3031:G:O6	2.32	0.45
36:m:65:ILE:HG12	36:m:74:VAL:HG22	1.99	0.45
45:a:346:SER:HB2	45:a:564:VAL:HG13	1.98	0.45
46:e:1270:TRP:NE1	46:e:1332:ILE:HD12	2.30	0.45
46:e:1272:TRP:NE1	46:e:1303:MET:HE3	2.31	0.45
31:h:7:G:OP1	36:m:33:ARG:NH1	2.48	0.45
46:e:294:SER:HA	46:e:297:HIS:ND1	2.31	0.45
46:e:409:PHE:CE2	46:e:425:VAL:HA	2.51	0.45
46:e:779:ALA:HB1	46:e:798:LEU:HD13	1.97	0.45
46:e:867:PHE:HB3	46:e:916:VAL:HG22	1.98	0.45
46:e:995:GLN:HE21	46:e:998:LYS:HE3	1.82	0.45
46:e:1477:GLN:O	46:e:1480:ILE:HG13	2.17	0.45
49:y:76:A:HO3'	52:1:57:UNK:C	2.12	0.45
29:d:21:ARG:HA	29:d:21:ARG:HD2	1.80	0.45
30:f:3116:G:OP1	30:f:3116:G:N2	2.43	0.45
36:m:83:LEU:HB3	36:m:88:ILE:HB	1.98	0.45
37:n:175:LYS:O	44:u:117:ARG:NH2	2.50	0.45
30:f:307:A:H2'	30:f:308:A:C8	2.52	0.45
30:f:1119:C:H2'	30:f:1120:A:H8	1.81	0.45
30:f:2697:A:H2'	30:f:2698:G:C8	2.52	0.45
33:j:140:ASN:O	33:j:144:ASN:HA	2.16	0.45
46:e:799:THR:HB	46:e:1094:TYR:CZ	2.51	0.45
46:e:856:ASN:HB3	46:e:859:TYR:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:e:1102:CYS:SG	46:e:1103:LEU:N	2.90	0.45
4:D:180:ARG:HH22	30:f:2719:U:H5''	1.82	0.45
23:W:30:GLN:NE2	30:f:904:A:OP2	2.50	0.45
30:f:1134:G:O2'	30:f:2642:A:N3	2.44	0.45
30:f:1497:C:H2'	30:f:1498:A:H8	1.81	0.45
31:h:62:U:O2'	36:m:285:ARG:NH2	2.50	0.45
33:j:14:SER:OG	33:j:15:ILE:N	2.50	0.45
33:j:104:LEU:HD12	33:j:158:ILE:HD11	1.98	0.45
46:e:133:ILE:HG21	46:e:173:PHE:CD2	2.52	0.45
46:e:809:MET:HB3	46:e:844:LEU:HD21	1.98	0.45
46:e:1213:TYR:HA	46:e:1238:PHE:CE1	2.51	0.45
30:f:448:U:O2	30:f:488:U:O2'	2.33	0.45
30:f:571:U:H2'	30:f:572:A:H8	1.81	0.45
38:o:83:LEU:HD11	38:o:116:PHE:HB3	1.99	0.45
45:a:199:ILE:HG12	45:a:212:LYS:HE3	1.99	0.45
46:e:314:LEU:HD23	46:e:361:LEU:CD2	2.37	0.45
30:f:2094:C:H2'	30:f:2095:G:H8	1.81	0.45
35:l:8:VAL:HG23	35:l:151:VAL:HG12	1.98	0.45
40:q:41:ILE:HD13	40:q:71:VAL:HB	1.99	0.45
46:e:662:ALA:HB1	46:e:668:VAL:HA	1.99	0.45
46:e:921:ILE:O	46:e:924:VAL:HG12	2.17	0.45
46:e:1188:ILE:H	46:e:1188:ILE:HG13	1.54	0.45
46:e:1244:LEU:HD21	46:e:1274:LEU:HB3	1.99	0.45
49:x:15:G:H22	49:x:48:C:H42	1.64	0.45
22:V:53:TYR:HA	22:V:56:ARG:HG2	1.99	0.45
30:f:528:U:H2'	30:f:529:A:C8	2.51	0.45
38:o:232:ARG:O	38:o:235:PHE:N	2.48	0.45
46:e:263:THR:HA	46:e:266:ARG:HD3	1.99	0.45
30:f:520:U:O4	35:l:347:THR:OG1	2.34	0.44
46:e:1027:ILE:O	46:e:1031:ILE:HG13	2.17	0.44
25:Y:37:TYR:O	30:f:351:A:N6	2.48	0.44
46:e:759:ASP:O	46:e:763:ILE:HG12	2.17	0.44
1:A:7:LEU:HD11	39:p:162:LEU:HA	1.99	0.44
30:f:2660:G:OP1	30:f:2750:U:O2'	2.35	0.44
30:f:2964:G:N2	30:f:2967:A:OP2	2.41	0.44
39:p:95:ASN:OD1	39:p:98:ARG:NH2	2.51	0.44
40:q:120:ASP:OD1	40:q:120:ASP:N	2.44	0.44
45:a:412:GLN:CG	46:e:5:GLY:HA3	2.47	0.44
46:e:314:LEU:HD22	46:e:358:VAL:HA	1.99	0.44
46:e:780:ILE:H	46:e:798:LEU:HD12	1.82	0.44
34:k:215:ILE:HD12	34:k:338:LEU:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:a:704:LEU:HD23	45:a:938:ILE:HD11	2.00	0.44
50:z:55:GLY:O	50:z:56:ILE:C	2.58	0.44
9:I:38:ALA:HB3	9:I:59:MET:HB2	1.99	0.44
30:f:1786:G:H2'	30:f:1787:A:C8	2.52	0.44
45:a:404:LEU:HD23	45:a:404:LEU:HA	1.90	0.44
46:e:96:ALA:O	46:e:99:ILE:HG12	2.18	0.44
46:e:367:ARG:HE	46:e:367:ARG:HB2	1.58	0.44
47:v:27:ARG:NH1	49:y:5:G:OP1	2.50	0.44
49:x:60:U:H5''	49:x:61:C:H5	1.83	0.44
30:f:19:U:H2'	30:f:20:A:C8	2.52	0.44
30:f:1203:A:N3	30:f:2855:U:O2'	2.46	0.44
30:f:1899:G:O2'	30:f:2334:U:O4	2.25	0.44
30:f:2284:C:N4	30:f:2308:C:OP2	2.50	0.44
30:f:2676:A:OP1	45:a:652:LYS:NZ	2.46	0.44
30:f:2960:C:H2'	30:f:2961:G:C8	2.53	0.44
30:f:3379:C:H4'	34:k:315:GLY:HA2	1.98	0.44
33:j:101:VAL:HG22	33:j:165:VAL:HG22	2.00	0.44
33:j:135:ILE:HD12	33:j:149:ARG:HE	1.82	0.44
46:e:716:ALA:O	46:e:723:ALA:HB2	2.17	0.44
46:e:1080:LEU:HD21	46:e:1106:TYR:HA	1.98	0.44
47:v:30:GLY:H	47:v:41:ILE:HG22	1.82	0.44
2:B:74[A]:ARG:NH1	30:f:3008:A:OP2	2.51	0.44
12:L:112:ASP:OD2	32:i:85:G:N1	2.49	0.44
24:X:10:GLN:HA	24:X:13:GLU:HG2	1.99	0.44
30:f:1888:U:H5''	34:k:247:ARG:HB2	2.00	0.44
36:m:205:SER:HB3	36:m:236:LEU:HD21	2.00	0.44
46:e:292:LEU:HB3	46:e:338:LYS:HD3	1.99	0.44
46:e:993:VAL:O	46:e:997:PHE:HB3	2.18	0.44
6:F:80:ARG:HG3	6:F:124:LEU:HD21	1.99	0.44
9:I:129:VAL:O	9:I:133:SER:HB3	2.17	0.44
14:N:36:GLY:HA3	14:N:40:HIS:CE1	2.53	0.44
30:f:799:G:O2'	43:t:18:TRP:NE1	2.47	0.44
30:f:2357:A:H2'	30:f:2358:A:C8	2.53	0.44
41:r:184:LYS:HB2	41:r:184:LYS:HE2	1.86	0.44
46:e:320:LEU:HB3	46:e:328:ILE:HD13	2.00	0.44
46:e:953:ASP:O	46:e:956:LEU:HB2	2.18	0.44
2:B:127[A]:LEU:HD22	6:F:156:VAL:HG13	2.00	0.44
7:G:68:THR:OG1	7:G:69:LYS:N	2.51	0.44
17:Q:46:THR:HG22	17:Q:48:ASP:H	1.82	0.44
30:f:911:C:OP1	33:j:14:SER:OG	2.32	0.44
31:h:38:U:N3	31:h:41:G:OP2	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:74:ILE:HD12	35:l:75:PRO:HD2	2.00	0.44
39:p:104:GLU:HA	39:p:107:GLU:HG3	2.00	0.44
46:e:796:LEU:CD2	46:e:797:LEU:HD23	2.42	0.44
46:e:1236:SER:HA	46:e:1239:LYS:HG2	2.00	0.44
6:F:80:ARG:HD2	7:G:155:PRO:HA	2.00	0.43
15:O:14:ARG:NH2	30:f:1139:G:OP2	2.51	0.43
22:V:9:ILE:HD12	43:t:174:ARG:HB2	1.99	0.43
23:W:63:ARG:NH1	32:i:58:G:O6	2.50	0.43
30:f:595:G:OP2	38:o:30:ARG:NH1	2.51	0.43
30:f:1657:C:O2'	30:f:1797:A:OP2	2.30	0.43
30:f:1764:U:H3'	30:f:1765:U:C4'	2.44	0.43
30:f:2116:G:OP1	30:f:2118:C:N4	2.51	0.43
30:f:3322:A:H2'	30:f:3323:A:C8	2.53	0.43
46:e:244:GLU:HA	46:e:247:TRP:CD1	2.53	0.43
7:G:133:ALA:HB3	38:o:121:LYS:HB2	2.00	0.43
30:f:710:A:H2'	30:f:711:A:C8	2.54	0.43
46:e:1377:ARG:H	46:e:1377:ARG:HG3	1.33	0.43
48:w:37:GLY:O	48:w:202:GLY:N	2.52	0.43
48:w:96:ASN:HD21	48:w:99:LEU:HD12	1.83	0.43
8:H:20:SER:HA	8:H:23:THR:HG22	2.00	0.43
23:W:58:THR:OG1	23:W:59:THR:N	2.51	0.43
30:f:1222:G:N2	30:f:1285:G:O2'	2.51	0.43
30:f:1259:A:N3	30:f:1280:C:O2'	2.50	0.43
30:f:1813:A:O2'	30:f:1816:A:N3	2.46	0.43
30:f:2768:U:H2'	30:f:2769:A:H8	1.83	0.43
30:f:2875:U:H3	52:1:56:UNK:HA	1.83	0.43
30:f:3016:A:H2'	30:f:3017:A:H8	1.83	0.43
30:f:3295:A:H2'	30:f:3296:A:C8	2.53	0.43
46:e:822:LEU:HA	46:e:822:LEU:HD23	1.56	0.43
51:O:45:LEU:HB3	51:O:49:ALA:HB3	1.99	0.43
20:T:95:ILE:HG21	20:T:95:ILE:HD13	1.81	0.43
30:f:1237:G:H22	30:f:1251:A:H2	1.66	0.43
39:p:82:LEU:HD13	39:p:222:PHE:HE2	1.84	0.43
45:a:117:PHE:CD1	45:a:118:SER:N	2.86	0.43
46:e:770:ILE:HD13	46:e:901:SER:HB2	2.01	0.43
46:e:776:TYR:HB3	46:e:812:LEU:HB2	2.00	0.43
46:e:782:TYR:HA	46:e:785:SER:HB3	2.01	0.43
4:D:161:LYS:HA	4:D:161:LYS:HD3	1.82	0.43
9:I:117:PRO:HA	9:I:135:VAL:HG13	2.00	0.43
36:m:258:LYS:O	36:m:265:TYR:OH	2.31	0.43
39:p:86:THR:HA	39:p:89:GLU:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:p:239:GLY:O	39:p:243:GLN:HB2	2.19	0.43
46:e:783:ARG:HE	46:e:783:ARG:HB3	1.45	0.43
46:e:1192:ARG:HD2	46:e:1270:TRP:CZ2	2.53	0.43
51:0:15:LEU:O	51:0:19:LEU:HG	2.18	0.43
23:W:27:PHE:HA	23:W:34:CYS:HA	2.01	0.43
30:f:1666:G:H2'	30:f:1667:A:H8	1.83	0.43
30:f:2514:U:H5'	39:p:68:ARG:HG3	2.00	0.43
46:e:72:LEU:HB3	46:e:79:ASN:HD21	1.82	0.43
46:e:378:LEU:HB3	46:e:379:PRO:HD3	2.01	0.43
49:x:41:G:H2'	49:x:42:A:C8	2.54	0.43
4:D:124:LEU:HD13	4:D:127:LEU:HD23	2.01	0.43
6:F:70:THR:OG1	44:u:55:ARG:NH1	2.51	0.43
24:X:2:ALA:N	24:X:51:LEU:O	2.52	0.43
30:f:1288:U:H2'	30:f:1289:G:C8	2.54	0.43
30:f:2836:C:H5	30:f:2852:C:H42	1.67	0.43
46:e:1047:THR:O	46:e:1051:LEU:HG	2.18	0.43
46:e:1192:ARG:HD3	46:e:1192:ARG:HA	1.18	0.43
1:A:12:ARG:NH1	30:f:297:G:O6	2.46	0.43
1:A:68:ARG:HA	1:A:98:LEU:HD21	2.01	0.43
28:c:66:GLY:HA2	33:j:80:GLU:HG3	2.01	0.43
30:f:716:A:OP1	30:f:752:C:O2'	2.37	0.43
30:f:1675:G:H2'	30:f:1676:A:H8	1.83	0.43
30:f:2218:G:H2'	30:f:2219:A:C8	2.54	0.43
49:y:68:C:H2'	49:y:69:G:C8	2.53	0.43
51:0:75:LYS:O	51:0:78:PRO:HD2	2.19	0.43
1:A:158:HIS:HB3	1:A:161:ALA:HB3	2.00	0.43
3:C:56:ARG:NH2	3:C:75:GLU:OE2	2.51	0.43
5:E:102:LEU:HD22	5:E:138:LEU:HD22	2.01	0.43
10:J:34:SER:OG	30:f:3085:G:OP1	2.32	0.43
18:R:3:SER:OG	18:R:4:LEU:N	2.51	0.43
30:f:2129:U:H2'	30:f:2130:G:C8	2.54	0.43
30:f:2514:U:OP2	30:f:2586:G:N2	2.50	0.43
30:f:2745:G:N2	30:f:2748:A:OP2	2.47	0.43
30:f:3121:U:H1'	30:f:3122:A:H5''	2.01	0.43
30:f:3358:U:H2'	30:f:3359:A:H8	1.84	0.43
33:j:46:LYS:HD2	33:j:46:LYS:HA	1.81	0.43
45:a:391:LEU:HD23	45:a:391:LEU:HA	1.87	0.43
47:v:80:MET:HE3	47:v:80:MET:HB3	1.75	0.43
3:C:179:GLN:HA	3:C:182:ILE:HG22	2.00	0.43
23:W:45:ARG:NH2	30:f:361:A:O3'	2.52	0.43
44:u:93:LYS:HE3	44:u:93:LYS:HB2	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:e:146:SER:O	46:e:150:PRO:HD2	2.19	0.43
46:e:284:MET:HE1	46:e:323:TYR:CE2	2.54	0.43
46:e:1002:LEU:HD23	46:e:1002:LEU:HA	1.72	0.43
48:w:43:PRO:HD3	48:w:163:LEU:HD21	2.01	0.43
2:B:54[A]:TYR:OH	2:B:73[A]:PHE:O	2.37	0.42
30:f:2213:A:H2'	30:f:2214:A:C8	2.54	0.42
30:f:2747:A:H2'	30:f:2748:A:C8	2.54	0.42
46:e:238:LYS:HB2	46:e:238:LYS:HE2	1.65	0.42
46:e:1535:HIS:HB2	46:e:1538:CYS:SG	2.58	0.42
6:F:95:ARG:HB2	6:F:140:VAL:HG23	2.00	0.42
12:L:86:THR:OG1	12:L:94:SER:OG	2.36	0.42
41:r:72:ALA:HB2	41:r:155:ALA:HB2	2.01	0.42
45:a:54:VAL:HG22	45:a:60:ILE:HG13	2.00	0.42
46:e:16:LEU:HB2	46:e:19:GLY:O	2.19	0.42
46:e:716:ALA:HB1	46:e:723:ALA:HA	2.01	0.42
46:e:911:ARG:O	46:e:915:LYS:HG2	2.19	0.42
46:e:961:LEU:HB3	46:e:1005:ASN:HB3	2.01	0.42
46:e:992:LEU:HD13	46:e:1034:TRP:CZ2	2.54	0.42
46:e:1099:ARG:HH12	46:e:1142:GLU:HB2	1.84	0.42
4:D:36:LEU:O	4:D:40:THR:OG1	2.27	0.42
21:U:78:LYS:HA	21:U:81:ARG:HG2	2.00	0.42
27:b:28:TYR:HB3	27:b:69:VAL:HB	2.01	0.42
28:c:44:LYS:NZ	30:f:1727:G:OP1	2.51	0.42
30:f:417:A:H2'	30:f:418:A:C8	2.54	0.42
30:f:2442:G:H2'	30:f:2443:A:H8	1.83	0.42
34:k:83:PRO:O	34:k:165:GLN:NE2	2.47	0.42
36:m:6:ASP:OD1	36:m:6:ASP:N	2.48	0.42
44:u:47:ASP:HB2	44:u:55:ARG:HG3	2.02	0.42
45:a:117:PHE:HD1	45:a:118:SER:O	2.02	0.42
45:a:549:LYS:HA	45:a:549:LYS:HD3	1.73	0.42
46:e:932:LEU:HA	46:e:935:SER:HB2	2.01	0.42
46:e:1104:ASN:O	46:e:1107:GLU:HG3	2.19	0.42
46:e:1213:TYR:HD1	46:e:1238:PHE:CD2	2.36	0.42
46:e:1279:PHE:CZ	46:e:1290:PHE:HB3	2.54	0.42
6:F:32:SER:HB2	6:F:36:ILE:HD12	2.00	0.42
30:f:2160:G:H2'	30:f:2161:G:H8	1.84	0.42
30:f:3233:C:H2'	30:f:3234:A:C8	2.55	0.42
36:m:200:PHE:HB3	36:m:237:GLU:HG2	2.01	0.42
42:s:96:PHE:HB2	42:s:156:LYS:HE3	2.01	0.42
45:a:967:LEU:HD13	45:a:1005:LEU:HB2	2.01	0.42
46:e:43:TYR:CD2	46:e:82:PHE:HA	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:e:241:LEU:HA	46:e:246:ILE:HD11	2.01	0.42
49:x:68:C:H2'	49:x:69:G:C8	2.54	0.42
51:0:14:LYS:HE3	51:0:52:LEU:HD11	2.00	0.42
8:H:41:ILE:HG21	8:H:54:VAL:HG21	2.02	0.42
9:I:80:ARG:HB2	9:I:99:ALA:HB3	2.00	0.42
30:f:760:G:O2'	30:f:770:G:N2	2.43	0.42
30:f:1666:G:H2'	30:f:1667:A:C8	2.54	0.42
30:f:3023:U:H2'	30:f:3024:A:H8	1.84	0.42
45:a:601:TYR:HA	45:a:605:ILE:HB	2.02	0.42
46:e:355:PHE:HB2	46:e:404:GLU:HG2	2.01	0.42
46:e:710:LYS:HA	46:e:710:LYS:HD3	1.82	0.42
46:e:1033:LYS:HE2	46:e:1033:LYS:HB3	1.77	0.42
51:0:67:LEU:HD22	51:0:67:LEU:HA	1.85	0.42
51:0:70:LEU:HB3	51:0:73:PHE:CD1	2.55	0.42
6:F:137:ARG:HH21	30:f:1213:G:H5'	1.85	0.42
18:R:45:ARG:O	30:f:1145:G:O2'	2.36	0.42
22:V:18:THR:HG23	43:t:106:GLN:HB3	2.02	0.42
27:b:10:THR:HG21	27:b:72:LEU:HD13	2.01	0.42
30:f:673:U:H2'	30:f:674:G:C8	2.55	0.42
30:f:1203:A:H2'	30:f:1204:A:C8	2.55	0.42
30:f:1579:C:H2'	30:f:1580:A:C8	2.55	0.42
39:p:183:LYS:HB2	39:p:194:THR:HG23	2.01	0.42
45:a:840:LYS:HA	45:a:840:LYS:HD3	1.91	0.42
46:e:161:LYS:HB2	46:e:161:LYS:HE3	1.83	0.42
46:e:314:LEU:HB2	46:e:357:ALA:HB1	2.01	0.42
30:f:3016:A:H2'	30:f:3017:A:C8	2.55	0.42
46:e:377:TRP:HB3	46:e:412:PHE:CE1	2.55	0.42
46:e:866:PHE:HE2	46:e:916:VAL:HG21	1.85	0.42
46:e:1068:MET:HE3	46:e:1068:MET:HB3	1.94	0.42
1:A:90:ASN:ND2	30:f:2424:A:OP1	2.50	0.42
3:C:182:ILE:HD12	3:C:182:ILE:HA	1.85	0.42
16:P:73:GLY:N	16:P:76:GLU:OE1	2.42	0.42
30:f:158:G:H2'	30:f:159:A:H8	1.85	0.42
34:k:214:MET:HE3	34:k:214:MET:HB3	1.94	0.42
45:a:45:LYS:HG2	45:a:46:PRO:HD2	2.01	0.42
45:a:893:LYS:HA	45:a:893:LYS:HD3	1.48	0.42
46:e:237:LEU:HD23	46:e:237:LEU:HA	1.88	0.42
46:e:409:PHE:HE2	46:e:425:VAL:HA	1.84	0.42
46:e:593:PHE:O	46:e:594:ASN:C	2.62	0.42
46:e:746:TYR:HB3	46:e:818:PHE:CE1	2.55	0.42
46:e:780:ILE:HG13	46:e:798:LEU:HD12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:e:987:ILE:CG2	46:e:992:LEU:HB2	2.50	0.42
46:e:1461:ARG:HG3	46:e:1469:TRP:CG	2.55	0.42
47:v:51:5CT:H5	47:v:52:HIS:CE1	2.55	0.42
24:X:33:LYS:HA	24:X:33:LYS:HD3	1.84	0.42
27:b:10:THR:HA	27:b:20:HIS:HD2	1.84	0.42
35:l:276:LEU:HD23	35:l:276:LEU:HA	1.91	0.42
36:m:95:TRP:CE3	36:m:198:TYR:HB3	2.54	0.42
36:m:144:VAL:HG11	36:m:171:LEU:HD13	2.02	0.42
46:e:396:ARG:HA	46:e:397:ASN:HA	1.83	0.42
46:e:1084:LEU:HD13	46:e:1084:LEU:HA	1.65	0.42
46:e:1106:TYR:CD1	46:e:1127:ILE:HG21	2.55	0.42
30:f:129:U:H2'	30:f:130:A:C8	2.54	0.42
30:f:296:A:N3	30:f:299:G:O2'	2.53	0.42
30:f:1194:G:H2'	30:f:1195:A:C8	2.55	0.42
30:f:1660:C:H2'	30:f:1661:G:H8	1.85	0.42
30:f:2413:A:H2'	30:f:2414:G:H8	1.85	0.42
30:f:2923:U:O4	49:x:74:C:N3	2.52	0.42
34:k:106:TRP:O	34:k:137:TYR:OH	2.24	0.42
35:l:261:VAL:HG23	35:l:262:TRP:CD1	2.55	0.42
36:m:266:ALA:O	36:m:270:LYS:HB2	2.20	0.42
45:a:113:VAL:HB	45:a:123:ILE:HB	2.01	0.42
46:e:894:LEU:HD23	46:e:894:LEU:HA	1.86	0.42
46:e:1276:LEU:HD13	46:e:1358:GLN:HG2	2.02	0.42
3:C:116:HIS:HB3	3:C:149:VAL:HB	2.02	0.41
16:P:29:SER:OG	30:f:1730:G:O6	2.37	0.41
30:f:2772:C:H4'	30:f:2773:C:H5'	2.02	0.41
30:f:2852:C:N3	41:r:158:LYS:NZ	2.68	0.41
30:f:3163:A:N6	30:f:3288:G:O6	2.53	0.41
20:T:60:ARG:NH1	30:f:1593:A:OP1	2.53	0.41
27:b:61:LYS:NZ	27:b:63:LYS:O	2.53	0.41
30:f:443:G:O6	30:f:490:C:N4	2.53	0.41
30:f:531:G:H2'	30:f:532:A:C8	2.55	0.41
30:f:2451:G:H2'	30:f:2452:G:C8	2.55	0.41
30:f:2711:C:O2'	30:f:2744:U:OP1	2.38	0.41
35:l:6:VAL:N	35:l:20:LEU:O	2.48	0.41
37:n:112:THR:HG23	37:n:115:GLU:H	1.85	0.41
46:e:303:ILE:HD12	46:e:303:ILE:HA	1.83	0.41
46:e:306:VAL:O	46:e:309:VAL:HG12	2.20	0.41
46:e:404:GLU:O	46:e:408:ASN:ND2	2.53	0.41
46:e:770:ILE:CG1	46:e:898:ILE:HG23	2.48	0.41
46:e:989:GLU:HA	46:e:1034:TRP:CD1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:LEU:HD22	1:A:128:LYS:HD2	2.02	0.41
12:L:63:LYS:HA	12:L:63:LYS:HD3	1.92	0.41
30:f:596:C:N3	30:f:608:A:O2'	2.54	0.41
30:f:1577:G:H2'	30:f:1578:C:H6	1.85	0.41
30:f:3198:U:H1'	40:q:21:LYS:HB2	2.01	0.41
46:e:355:PHE:CD2	46:e:405:PHE:HB2	2.55	0.41
6:F:110:MET:HE3	6:F:110:MET:HB3	1.95	0.41
30:f:675:C:O2'	30:f:679:U:OP1	2.34	0.41
30:f:1221:A:C4	51:0:12:PHE:HZ	2.37	0.41
30:f:3218:A:H5''	30:f:3219:G:C5	2.55	0.41
42:s:55:ARG:O	42:s:58:GLY:N	2.53	0.41
46:e:292:LEU:CD1	46:e:332:ASP:HB3	2.50	0.41
46:e:1410:LEU:HD12	46:e:1410:LEU:HA	1.91	0.41
7:G:88:ARG:O	30:f:2722:U:O2'	2.35	0.41
30:f:20:A:H2'	30:f:21:G:C8	2.56	0.41
30:f:745:C:H2'	30:f:746:A:H8	1.85	0.41
30:f:2205:U:O4	45:a:854:GLN:NE2	2.42	0.41
35:l:343:LYS:HE2	35:l:343:LYS:HB2	1.92	0.41
46:e:281:LYS:H	46:e:281:LYS:HG3	1.57	0.41
46:e:1016:PHE:HD2	46:e:1062:PHE:HE2	1.67	0.41
49:x:34:I:H2'	49:x:35:G:C8	2.56	0.41
3:C:128:ARG:HB2	3:C:136:ILE:CG2	2.50	0.41
7:G:102:ARG:HD2	7:G:102:ARG:HA	1.76	0.41
26:Z:100:TYR:OH	30:f:2848:G:OP1	2.29	0.41
30:f:1497:C:H2'	30:f:1498:A:C8	2.56	0.41
31:h:53:U:O2'	31:h:55:A:N7	2.52	0.41
41:r:52:LEU:HB3	41:r:136:PHE:HB2	2.02	0.41
44:u:113:THR:OG1	44:u:114:ASP:N	2.52	0.41
46:e:177:LEU:O	46:e:181:VAL:HG23	2.20	0.41
46:e:1163:GLU:HB2	46:e:1166:LYS:HE3	2.03	0.41
46:e:1235:ASN:HD22	46:e:1235:ASN:HA	1.54	0.41
27:b:100:LYS:HE3	27:b:100:LYS:HB3	1.90	0.41
30:f:689:U:O4	35:l:209:TYR:OH	2.35	0.41
30:f:1421:G:H2'	30:f:1422:G:H8	1.86	0.41
34:k:284:ARG:HB3	34:k:323:MET:HB3	2.01	0.41
40:q:9:GLN:HB3	40:q:52:LEU:HD11	2.01	0.41
43:t:57:VAL:HG23	43:t:147:ILE:HD12	2.03	0.41
46:e:137:LEU:HD23	46:e:137:LEU:HA	1.90	0.41
46:e:290:LYS:HD2	46:e:290:LYS:HA	1.86	0.41
46:e:1461:ARG:HG3	46:e:1469:TRP:CD1	2.56	0.41
47:v:48:LYS:HD2	47:v:55:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8[A]:VAL:HG12	2:B:117[A]:ARG:HG3	2.03	0.41
22:V:5:THR:HG23	22:V:12:ASN:HB2	2.03	0.41
30:f:352:A:H61	30:f:365:A:H5''	1.86	0.41
46:e:981:ALA:HB1	46:e:1027:ILE:HD11	2.03	0.41
46:e:1491:LEU:HD23	46:e:1491:LEU:HA	1.92	0.41
48:w:122:ARG:HA	48:w:122:ARG:HD2	1.64	0.41
48:w:204:LEU:HB2	48:w:216:LEU:O	2.21	0.41
1:A:9:GLU:HG3	22:V:44:VAL:HG21	2.03	0.41
1:A:155:VAL:HG12	30:f:58:G:H4'	2.03	0.41
3:C:122:ALA:HB3	3:C:143:PRO:HB2	2.02	0.41
3:C:131:ARG:HG3	3:C:137:ASN:ND2	2.36	0.41
14:N:75:LEU:HD23	14:N:75:LEU:HA	1.92	0.41
14:N:114:GLY:O	14:N:137:LYS:NZ	2.54	0.41
18:R:99:ASN:O	30:f:1388:U:O2'	2.36	0.41
30:f:63:A:N3	30:f:78:U:O2'	2.43	0.41
30:f:1083:G:H2'	30:f:1084:A:C8	2.56	0.41
30:f:3092:C:O2'	30:f:3094:A:OP2	2.28	0.41
35:l:34:ILE:HG21	35:l:120:TYR:HD2	1.85	0.41
41:r:44:ASP:OD1	41:r:44:ASP:N	2.48	0.41
42:s:75:LYS:O	42:s:79:ILE:HG13	2.21	0.41
45:a:246:ASP:HB2	45:a:249:GLU:HB2	2.02	0.41
45:a:597:THR:HG23	45:a:621:TRP:HE1	1.86	0.41
45:a:702:GLY:HA2	45:a:952:TYR:O	2.21	0.41
45:a:893:LYS:HZ1	47:v:129:ASP:C	2.29	0.41
46:e:277:MET:HB2	46:e:278:PRO:HD3	2.03	0.41
46:e:378:LEU:HA	46:e:412:PHE:HZ	1.85	0.41
46:e:959:ILE:H	46:e:959:ILE:HG13	1.51	0.41
46:e:1299:LEU:HD12	46:e:1299:LEU:HA	1.77	0.41
1:A:18:VAL:HG13	1:A:19:LEU:HD12	2.02	0.41
6:F:43:TYR:OH	31:h:96:U:OP1	2.35	0.41
6:F:90:MET:HE3	30:f:1213:G:H4'	2.03	0.41
18:R:4:LEU:HD12	18:R:5:PRO:HD2	2.02	0.41
23:W:31:LYS:NZ	30:f:815:G:OP2	2.52	0.41
30:f:1660:C:H2'	30:f:1661:G:C8	2.56	0.41
30:f:2357:A:H2'	30:f:2358:A:H8	1.85	0.41
30:f:3217:C:C5	30:f:3220:G:H1'	2.56	0.41
31:h:84:A:H2'	31:h:85:G:C8	2.56	0.41
45:a:601:TYR:HA	45:a:605:ILE:HD12	2.03	0.41
46:e:987:ILE:HG23	46:e:992:LEU:HB2	2.03	0.41
46:e:1012:ALA:HB1	46:e:1062:PHE:HA	2.03	0.41
46:e:1371:TRP:HB2	46:e:1451:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:v:96:ASP:OD1	47:v:96:ASP:N	2.54	0.41
48:w:151:VAL:O	48:w:154:THR:OG1	2.33	0.41
49:y:62:C:H2'	49:y:63:G:C8	2.55	0.41
8:H:25:ASN:ND2	8:H:107:PHE:CD2	2.90	0.40
30:f:2470:C:OP1	48:w:27:ASN:N	2.47	0.40
40:q:90:MET:HE3	40:q:179:ILE:HG22	2.01	0.40
41:r:144:ASN:HD22	41:r:144:ASN:N	2.18	0.40
41:r:181:TYR:CE2	41:r:185:ARG:HD2	2.56	0.40
49:x:68:C:H2'	49:x:69:G:H8	1.86	0.40
1:A:174:ILE:HG21	30:f:63:A:H5''	2.04	0.40
2:B:121[A]:PRO:HA	2:B:124[A]:LEU:HD12	2.03	0.40
8:H:19:VAL:HG12	8:H:105:LEU:HD13	2.02	0.40
12:L:51:ARG:NH2	32:i:83:C:O2	2.54	0.40
17:Q:20:LEU:HD11	17:Q:32:ALA:HB2	2.03	0.40
24:X:2:ALA:HB1	30:f:1747:G:H21	1.86	0.40
26:Z:113:ARG:NH2	30:f:1190:A:H4'	2.36	0.40
30:f:129:U:H3	30:f:139:G:H1	1.69	0.40
30:f:946:U:H2'	30:f:947:G:H8	1.86	0.40
30:f:1249:G:H2'	30:f:1250:G:H8	1.86	0.40
34:k:218:ILE:HG12	34:k:276:THR:HG23	2.03	0.40
36:m:108:ARG:CZ	36:m:253:PHE:HB2	2.51	0.40
46:e:746:TYR:HB3	46:e:818:PHE:HE1	1.86	0.40
46:e:1325:LYS:H	46:e:1325:LYS:HG2	1.67	0.40
2:B:189[A]:ASP:OD1	2:B:190[A]:VAL:N	2.53	0.40
4:D:155:MET:HE2	4:D:163:PRO:HB3	2.03	0.40
30:f:1238:C:C4'	50:z:139:VAL:CB	2.98	0.40
30:f:1596:C:H2'	30:f:1597:C:C6	2.56	0.40
33:j:52:SER:HB3	33:j:191:LEU:HD23	2.02	0.40
43:t:189:GLU:HA	43:t:192:GLU:HG3	2.03	0.40
46:e:377:TRP:HB3	46:e:412:PHE:HE1	1.86	0.40
46:e:823:LEU:HD22	46:e:830:VAL:HA	2.04	0.40
2:B:164[A]:SER:OG	30:f:3181:C:O2'	2.34	0.40
20:T:93:PHE:HD2	20:T:94:LEU:HD22	1.86	0.40
30:f:182:U:H2'	30:f:183:G:H8	1.86	0.40
30:f:1108:U:H2'	30:f:1109:U:C6	2.56	0.40
45:a:25:ARG:HD2	49:y:35:G:OP1	2.22	0.40
46:e:247:TRP:CZ2	46:e:283:ILE:HG23	2.56	0.40
46:e:698:TYR:HE2	46:e:746:TYR:CD1	2.40	0.40
46:e:1095:LEU:HA	46:e:1098:LEU:HD12	2.04	0.40
46:e:1164:LEU:H	46:e:1164:LEU:HD23	1.87	0.40
7:G:73:GLY:HA2	7:G:89:LEU:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:f:1799:A:H2'	30:f:1800:A:C8	2.57	0.40
30:f:1827:C:H2'	30:f:1828:A:C8	2.57	0.40
35:l:233:LEU:HD23	35:l:233:LEU:HA	1.90	0.40
45:a:5:ILE:HD12	45:a:59:ARG:HA	2.03	0.40
45:a:574:PHE:HB2	45:a:589:MET:HE1	2.02	0.40
46:e:216:VAL:HG13	46:e:267:LEU:HD22	2.03	0.40
46:e:305:LYS:O	46:e:308:PRO:HD2	2.22	0.40
46:e:933:LEU:HG	46:e:964:PHE:HD2	1.86	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	A	201/204 (98%)	190 (94%)	11 (6%)	0	100	100
2	B	195/199 (98%)	192 (98%)	3 (2%)	0	100	100
3	C	181/184 (98%)	172 (95%)	9 (5%)	0	100	100
4	D	183/186 (98%)	176 (96%)	7 (4%)	0	100	100
5	E	154/189 (82%)	151 (98%)	3 (2%)	0	100	100
6	F	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
7	G	157/160 (98%)	149 (95%)	8 (5%)	0	100	100
8	H	100/121 (83%)	95 (95%)	4 (4%)	1 (1%)	12	20
9	I	134/137 (98%)	132 (98%)	2 (2%)	0	100	100
10	J	61/155 (39%)	61 (100%)	0	0	100	100
11	K	119/142 (84%)	118 (99%)	1 (1%)	0	100	100
12	L	123/127 (97%)	119 (97%)	4 (3%)	0	100	100
13	M	133/136 (98%)	126 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	N	146/149 (98%)	136 (93%)	10 (7%)	0	100	100
15	O	56/59 (95%)	52 (93%)	3 (5%)	1 (2%)	6	9
16	P	94/105 (90%)	93 (99%)	1 (1%)	0	100	100
17	Q	107/113 (95%)	103 (96%)	4 (4%)	0	100	100
18	R	125/130 (96%)	123 (98%)	2 (2%)	0	100	100
19	S	104/107 (97%)	101 (97%)	3 (3%)	0	100	100
20	T	110/121 (91%)	108 (98%)	2 (2%)	0	100	100
21	U	117/120 (98%)	112 (96%)	5 (4%)	0	100	100
22	V	97/100 (97%)	93 (96%)	4 (4%)	0	100	100
23	W	79/88 (90%)	75 (95%)	4 (5%)	0	100	100
24	X	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
25	Y	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
26	Z	50/128 (39%)	47 (94%)	3 (6%)	0	100	100
27	b	101/106 (95%)	95 (94%)	6 (6%)	0	100	100
28	c	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
29	d	20/25 (80%)	19 (95%)	1 (5%)	0	100	100
33	j	244/254 (96%)	226 (93%)	18 (7%)	0	100	100
34	k	384/387 (99%)	363 (94%)	21 (6%)	0	100	100
35	l	359/362 (99%)	329 (92%)	29 (8%)	1 (0%)	36	50
36	m	292/297 (98%)	277 (95%)	15 (5%)	0	100	100
37	n	163/176 (93%)	154 (94%)	9 (6%)	0	100	100
38	o	220/244 (90%)	207 (94%)	13 (6%)	0	100	100
39	p	231/256 (90%)	220 (95%)	11 (5%)	0	100	100
40	q	189/191 (99%)	174 (92%)	14 (7%)	1 (0%)	24	37
41	r	216/221 (98%)	206 (95%)	10 (5%)	0	100	100
42	s	167/174 (96%)	161 (96%)	5 (3%)	1 (1%)	21	32
43	t	191/199 (96%)	174 (91%)	16 (8%)	1 (0%)	24	37
44	u	134/138 (97%)	125 (93%)	9 (7%)	0	100	100
45	a	842/1038 (81%)	826 (98%)	16 (2%)	0	100	100
46	e	1519/1562 (97%)	1497 (99%)	20 (1%)	2 (0%)	48	64
47	v	139/157 (88%)	139 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	w	214/217 (99%)	211 (99%)	3 (1%)	0	100	100
50	z	144/165 (87%)	136 (94%)	7 (5%)	1 (1%)	18	28
51	0	117/312 (38%)	116 (99%)	0	1 (1%)	14	22
All	All	9093/10034 (91%)	8747 (96%)	336 (4%)	10 (0%)	49	64

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
46	e	393	PHE
50	z	88	PRO
46	e	1339	PRO
8	H	91	ASP
35	l	4	PRO
40	q	107	ASP
42	s	108	GLU
51	0	93	LEU
15	O	21	ILE
43	t	47	ALA

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	A	175/176 (99%)	175 (100%)	0	100	100
2	B	160/162 (99%)	160 (100%)	0	100	100
3	C	138/146 (94%)	137 (99%)	1 (1%)	76	88
4	D	150/151 (99%)	150 (100%)	0	100	100
5	E	129/154 (84%)	129 (100%)	0	100	100
6	F	155/156 (99%)	155 (100%)	0	100	100
7	G	135/137 (98%)	135 (100%)	0	100	100
8	H	89/107 (83%)	87 (98%)	2 (2%)	45	67
9	I	104/105 (99%)	104 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	54/129 (42%)	54 (100%)	0	100	100
11	K	104/118 (88%)	104 (100%)	0	100	100
12	L	108/110 (98%)	108 (100%)	0	100	100
13	M	112/116 (97%)	112 (100%)	0	100	100
14	N	117/119 (98%)	117 (100%)	0	100	100
15	O	46/47 (98%)	46 (100%)	0	100	100
16	P	81/88 (92%)	81 (100%)	0	100	100
17	Q	92/97 (95%)	88 (96%)	4 (4%)	26	44
18	R	107/111 (96%)	107 (100%)	0	100	100
19	S	90/91 (99%)	90 (100%)	0	100	100
20	T	95/103 (92%)	95 (100%)	0	100	100
21	U	104/105 (99%)	104 (100%)	0	100	100
22	V	80/82 (98%)	80 (100%)	0	100	100
23	W	67/71 (94%)	67 (100%)	0	100	100
24	X	68/69 (99%)	68 (100%)	0	100	100
25	Y	45/46 (98%)	45 (100%)	0	100	100
26	Z	45/116 (39%)	45 (100%)	0	100	100
27	b	87/91 (96%)	87 (100%)	0	100	100
28	c	71/72 (99%)	71 (100%)	0	100	100
29	d	20/23 (87%)	20 (100%)	0	100	100
33	j	189/196 (96%)	189 (100%)	0	100	100
34	k	320/323 (99%)	320 (100%)	0	100	100
35	l	288/289 (100%)	288 (100%)	0	100	100
36	m	241/245 (98%)	241 (100%)	0	100	100
37	n	139/155 (90%)	139 (100%)	0	100	100
38	o	186/205 (91%)	186 (100%)	0	100	100
39	p	187/208 (90%)	187 (100%)	0	100	100
40	q	168/171 (98%)	168 (100%)	0	100	100
41	r	185/187 (99%)	184 (100%)	1 (0%)	81	91
42	s	145/150 (97%)	142 (98%)	3 (2%)	47	69
43	t	154/159 (97%)	154 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	u	107/109 (98%)	107 (100%)	0	100	100
45	a	678/949 (71%)	675 (100%)	3 (0%)	84	92
46	e	1150/1451 (79%)	1025 (89%)	125 (11%)	6	9
47	v	119/132 (90%)	118 (99%)	1 (1%)	73	86
48	w	197/198 (100%)	196 (100%)	1 (0%)	81	91
51	0	104/254 (41%)	94 (90%)	10 (10%)	8	12
All	All	7385/8479 (87%)	7234 (98%)	151 (2%)	48	70

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	128	ARG
8	H	93	ILE
8	H	105	LEU
17	Q	79	ARG
17	Q	81	GLU
17	Q	107	VAL
17	Q	108	VAL
41	r	112	GLN
42	s	29	ARG
42	s	55	ARG
42	s	60	ARG
45	a	98	ASP
45	a	136	ARG
45	a	893	LYS
46	e	16	LEU
46	e	18	LEU
46	e	21	ASN
46	e	23	VAL
46	e	28	ASN
46	e	35	ASP
46	e	57	ARG
46	e	72	LEU
46	e	105	VAL
46	e	114	THR
46	e	125	ILE
46	e	147	VAL
46	e	157	GLU
46	e	178	LEU
46	e	190	GLU

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Mol	Chain	Res	Type
46	e	205	GLU
46	e	212	ILE
46	e	239	VAL
46	e	246	ILE
46	e	251	ASN
46	e	264	VAL
46	e	281	LYS
46	e	283	ILE
46	e	299	THR
46	e	301	LYS
46	e	309	VAL
46	e	320	LEU
46	e	327	THR
46	e	342	PHE
46	e	345	VAL
46	e	358	VAL
46	e	375	LEU
46	e	404	GLU
46	e	705	ASN
46	e	736	VAL
46	e	751	VAL
46	e	753	LEU
46	e	761	SER
46	e	777	MET
46	e	782	TYR
46	e	783	ARG
46	e	787	VAL
46	e	794	THR
46	e	796	LEU
46	e	804	ILE
46	e	806	LEU
46	e	810	GLN
46	e	812	LEU
46	e	819	LEU
46	e	822	LEU
46	e	828	GLU
46	e	834	ILE
46	e	838	ILE
46	e	851	LEU
46	e	861	ASP
46	e	862	PHE
46	e	893	MET

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Mol	Chain	Res	Type
46	e	904	VAL
46	e	927	THR
46	e	928	THR
46	e	933	LEU
46	e	955	LEU
46	e	959	ILE
46	e	974	THR
46	e	979	LEU
46	e	987	ILE
46	e	992	LEU
46	e	993	VAL
46	e	997	PHE
46	e	1000	LEU
46	e	1003	LEU
46	e	1004	ASN
46	e	1006	LEU
46	e	1007	LEU
46	e	1009	ILE
46	e	1017	VAL
46	e	1019	ILE
46	e	1024	LEU
46	e	1039	LEU
46	e	1042	GLU
46	e	1047	THR
46	e	1053	LEU
46	e	1075	LEU
46	e	1077	GLU
46	e	1079	LEU
46	e	1080	LEU
46	e	1084	LEU
46	e	1092	THR
46	e	1093	LEU
46	e	1094	TYR
46	e	1095	LEU
46	e	1096	LEU
46	e	1099	ARG
46	e	1102	CYS
46	e	1123	TYR
46	e	1144	ASN
46	e	1147	VAL
46	e	1179	LEU
46	e	1184	ILE

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Mol	Chain	Res	Type
46	e	1188	ILE
46	e	1192	ARG
46	e	1202	VAL
46	e	1214	GLU
46	e	1235	ASN
46	e	1240	LEU
46	e	1269	LEU
46	e	1270	TRP
46	e	1332	ILE
46	e	1341	LYS
46	e	1342	GLU
46	e	1358	GLN
46	e	1359	LEU
46	e	1363	VAL
46	e	1367	THR
46	e	1372	LEU
46	e	1377	ARG
46	e	1421	LEU
46	e	1425	THR
46	e	1439	LEU
46	e	1454	ILE
46	e	1461	ARG
46	e	1480	ILE
46	e	1508	CYS
46	e	1514	ILE
46	e	1532	ASN
47	v	54	HIS
48	w	92	LYS
51	0	30	VAL
51	0	51	VAL
51	0	52	LEU
51	0	67	LEU
51	0	76	LEU
51	0	80	VAL
51	0	93	LEU
51	0	95	GLU
51	0	105	VAL
51	0	189	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	GLN
2	B	193[A]	GLN
3	C	55	GLN
3	C	97	ASN
4	D	5	HIS
5	E	150	GLN
7	G	66	ASN
7	G	149	GLN
8	H	25	ASN
8	H	87	ASN
8	H	88	GLN
8	H	101	ASN
8	H	109	GLN
11	K	65	GLN
11	K	85	GLN
13	M	122	HIS
13	M	127	ASN
14	N	38	GLN
15	O	12	GLN
15	O	17	HIS
17	Q	15	ASN
17	Q	21	HIS
18	R	35	GLN
18	R	49	ASN
20	T	61	GLN
21	U	16	GLN
21	U	59	ASN
21	U	99	GLN
23	W	12	HIS
23	W	13	ASN
25	Y	4	GLN
25	Y	20	ASN
27	b	3	ASN
27	b	102	GLN
33	j	211	HIS
34	k	139	GLN
34	k	198	HIS
34	k	224	HIS
35	l	5	GLN
35	l	196	ASN
35	l	213	ASN
35	l	316	ASN
38	o	64	GLN

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Mol	Chain	Res	Type
38	o	225	GLN
38	o	244	ASN
39	p	77	GLN
40	q	49	ASN
40	q	169	ASN
40	q	183	HIS
41	r	51	HIS
41	r	208	ASN
42	s	43	GLN
42	s	62	ASN
42	s	90	GLN
44	u	62	GLN
45	a	94	GLN
45	a	121	ASN
45	a	147	GLN
45	a	382	GLN
45	a	395	ASN
45	a	417	ASN
45	a	438	ASN
45	a	562	HIS
46	e	21	ASN
46	e	79	ASN
46	e	109	GLN
46	e	160	ASN
46	e	233	ASN
46	e	368	HIS
46	e	719	ASN
46	e	805	ASN
46	e	864	HIS
46	e	968	ASN
46	e	995	GLN
46	e	1004	ASN
46	e	1005	ASN
46	e	1138	ASN
46	e	1145	ASN
46	e	1180	ASN
46	e	1189	ASN
46	e	1190	GLN
46	e	1288	GLN
46	e	1358	GLN
46	e	1477	GLN
46	e	1478	HIS

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Mol	Chain	Res	Type
46	e	1532	ASN
47	v	52	HIS
47	v	78	HIS
47	v	125	GLN
51	0	36	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	f	3212/3395 (94%)	589 (18%)	0
31	h	120/121 (99%)	12 (10%)	0
32	i	157/158 (99%)	32 (20%)	0
49	x	70/76 (92%)	19 (27%)	0
49	y	69/76 (90%)	18 (26%)	0
All	All	3628/3826 (94%)	670 (18%)	0

All (670) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	f	6	A
30	f	13	A
30	f	14	U
30	f	26	A
30	f	40	A
30	f	43	A
30	f	49	A
30	f	59	G
30	f	60	A
30	f	65	A
30	f	66	A
30	f	92	G
30	f	99	A
30	f	109	A
30	f	110	G
30	f	111	C
30	f	116	A
30	f	120	G
30	f	121	A
30	f	122	A
30	f	133	U
30	f	134	U

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Mol	Chain	Res	Type
30	f	135	C
30	f	136	G
30	f	156	G
30	f	157	A
30	f	165	A
30	f	166	C
30	f	172	G
30	f	173	G
30	f	187	A
30	f	190	U
30	f	191	U
30	f	200	C
30	f	206	G
30	f	210	U
30	f	211	A
30	f	213	A
30	f	218	G
30	f	219	A
30	f	234	G
30	f	240	U
30	f	241	G
30	f	242	C
30	f	243	G
30	f	245	U
30	f	249	U
30	f	252	U
30	f	269	G
30	f	283	G
30	f	286	U
30	f	295	A
30	f	305	U
30	f	323	A
30	f	329	U
30	f	339	C
30	f	350	C
30	f	374	A
30	f	376	G
30	f	398	A
30	f	399	A
30	f	401	U
30	f	402	A
30	f	403	C

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Mol	Chain	Res	Type
30	f	421	G
30	f	422	A
30	f	439	C
30	f	440	A
30	f	441	U
30	f	442	G
30	f	443	G
30	f	445	G
30	f	446	U
30	f	447	U
30	f	448	U
30	f	450	G
30	f	487	U
30	f	488	U
30	f	489	U
30	f	490	C
30	f	494	G
30	f	518	G
30	f	520	U
30	f	521	A
30	f	523	A
30	f	535	G
30	f	536	U
30	f	543	C
30	f	544	C
30	f	546	C
30	f	547	G
30	f	548	G
30	f	551	A
30	f	552	G
30	f	555	U
30	f	557	A
30	f	559	A
30	f	578	A
30	f	579	G
30	f	589	A
30	f	597	G
30	f	604	G
30	f	608	A
30	f	609	G
30	f	611	A
30	f	620	U

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Mol	Chain	Res	Type
30	f	621	A
30	f	622	A
30	f	637	C
30	f	638	C
30	f	649	A
30	f	660	A
30	f	677	A
30	f	681	U
30	f	684	G
30	f	690	A
30	f	691	A
30	f	705	A
30	f	712	G
30	f	715	A
30	f	716	A
30	f	719	U
30	f	720	A
30	f	758	C
30	f	763	G
30	f	764	U
30	f	765	C
30	f	766	U
30	f	767	U
30	f	776	U
30	f	777	U
30	f	780	A
30	f	781	G
30	f	785	G
30	f	786	A
30	f	806	A
30	f	817	A
30	f	830	A
30	f	846	A
30	f	849	C
30	f	850	U
30	f	861	C
30	f	874	U
30	f	879	U
30	f	896	A
30	f	907	G
30	f	908	G
30	f	914	A

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Mol	Chain	Res	Type
30	f	916	G
30	f	917	A
30	f	920	A
30	f	921	A
30	f	924	G
30	f	925	A
30	f	937	G
30	f	944	C
30	f	959	C
30	f	960	U
30	f	981	U
30	f	982	C
30	f	991	G
30	f	994	G
30	f	1001	G
30	f	1002	A
30	f	1010	G
30	f	1015	U
30	f	1016	C
30	f	1017	C
30	f	1018	G
30	f	1021	G
30	f	1024	G
30	f	1025	A
30	f	1028	U
30	f	1036	A
30	f	1041	U
30	f	1047	A
30	f	1049	C
30	f	1063	G
30	f	1064	A
30	f	1065	A
30	f	1072	G
30	f	1081	U
30	f	1087	G
30	f	1093	A
30	f	1094	U
30	f	1095	U
30	f	1097	G
30	f	1098	A
30	f	1103	A
30	f	1104	G

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Mol	Chain	Res	Type
30	f	1117	G
30	f	1131	G
30	f	1144	U
30	f	1153	A
30	f	1159	A
30	f	1160	C
30	f	1177	G
30	f	1180	A
30	f	1181	U
30	f	1192	C
30	f	1193	A
30	f	1196	C
30	f	1197	A
30	f	1201	C
30	f	1202	A
30	f	1208	U
30	f	1217	A
30	f	1218	U
30	f	1219	C
30	f	1222	G
30	f	1225	A
30	f	1227	C
30	f	1235	U
30	f	1236	G
30	f	1238	C
30	f	1241	U
30	f	1242	G
30	f	1244	A
30	f	1245	A
30	f	1251	A
30	f	1252	A
30	f	1254	C
30	f	1258	U
30	f	1259	A
30	f	1263	A
30	f	1264	G
30	f	1265	U
30	f	1269	U
30	f	1272	C
30	f	1277	C
30	f	1278	A
30	f	1279	C

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Mol	Chain	Res	Type
30	f	1282	G
30	f	1285	G
30	f	1286	A
30	f	1287	A
30	f	1295	G
30	f	1307	G
30	f	1308	A
30	f	1309	U
30	f	1313	G
30	f	1330	A
30	f	1348	U
30	f	1349	G
30	f	1351	U
30	f	1352	A
30	f	1354	G
30	f	1355	A
30	f	1356	U
30	f	1357	G
30	f	1386	A
30	f	1392	G
30	f	1399	A
30	f	1400	G
30	f	1419	A
30	f	1434	G
30	f	1437	C
30	f	1446	A
30	f	1450	G
30	f	1481	A
30	f	1482	A
30	f	1483	G
30	f	1487	G
30	f	1488	G
30	f	1502	C
30	f	1508	C
30	f	1536	G
30	f	1539	A
30	f	1555	U
30	f	1556	C
30	f	1557	A
30	f	1560	G
30	f	1562	C
30	f	1563	C

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Mol	Chain	Res	Type
30	f	1566	A
30	f	1568	U
30	f	1569	U
30	f	1572	U
30	f	1573	G
30	f	1575	A
30	f	1576	G
30	f	1580	A
30	f	1581	C
30	f	1582	C
30	f	1583	A
30	f	1589	A
30	f	1590	G
30	f	1605	A
30	f	1607	U
30	f	1620	U
30	f	1629	U
30	f	1639	C
30	f	1642	A
30	f	1643	A
30	f	1645	U
30	f	1657	C
30	f	1683	A
30	f	1716	U
30	f	1717	U
30	f	1724	U
30	f	1725	C
30	f	1736	G
30	f	1741	A
30	f	1750	A
30	f	1751	G
30	f	1760	A
30	f	1762	C
30	f	1765	U
30	f	1766	G
30	f	1770	G
30	f	1775	G
30	f	1780	G
30	f	1797	A
30	f	1814	A
30	f	1816	A
30	f	1819	U

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Mol	Chain	Res	Type
30	f	1820	U
30	f	1821	U
30	f	1835	A
30	f	1839	A
30	f	1840	U
30	f	1841	A
30	f	1842	A
30	f	1846	C
30	f	1849	C
30	f	1850	A
30	f	1866	C
30	f	1867	A
30	f	1880	U
30	f	1881	A
30	f	1893	A
30	f	1906	G
30	f	1943	C
30	f	1952	G
30	f	1953	G
30	f	1954	G
30	f	2094	C
30	f	2101	C
30	f	2102	U
30	f	2111	G
30	f	2112	U
30	f	2113	A
30	f	2114	C
30	f	2121	G
30	f	2122	G
30	f	2131	A
30	f	2134	G
30	f	2140	U
30	f	2144	A
30	f	2158	A
30	f	2160	G
30	f	2169	G
30	f	2176	U
30	f	2201	G
30	f	2206	G
30	f	2207	A
30	f	2208	A
30	f	2209	U

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Mol	Chain	Res	Type
30	f	2222	A
30	f	2223	A
30	f	2225	U
30	f	2228	A
30	f	2249	G
30	f	2272	G
30	f	2273	G
30	f	2274	U
30	f	2281	A
30	f	2282	U
30	f	2288	G
30	f	2307	G
30	f	2308	C
30	f	2310	U
30	f	2313	A
30	f	2314	U
30	f	2315	G
30	f	2334	U
30	f	2335	G
30	f	2336	U
30	f	2373	A
30	f	2374	C
30	f	2375	G
30	f	2385	G
30	f	2388	U
30	f	2393	G
30	f	2397	A
30	f	2402	A
30	f	2403	G
30	f	2404	A
30	f	2411	U
30	f	2419	A
30	f	2437	G
30	f	2446	U
30	f	2447	A
30	f	2450	G
30	f	2461	A
30	f	2463	G
30	f	2464	U
30	f	2468	A
30	f	2469	G
30	f	2470	C

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Mol	Chain	Res	Type
30	f	2471	U
30	f	2472	U
30	f	2474	G
30	f	2479	C
30	f	2480	A
30	f	2484	A
30	f	2486	A
30	f	2487	U
30	f	2488	A
30	f	2494	A
30	f	2495	C
30	f	2496	C
30	f	2499	U
30	f	2501	U
30	f	2502	A
30	f	2503	G
30	f	2505	U
30	f	2514	U
30	f	2515	A
30	f	2522	G
30	f	2526	C
30	f	2531	C
30	f	2537	U
30	f	2538	U
30	f	2539	C
30	f	2540	A
30	f	2541	U
30	f	2542	U
30	f	2544	U
30	f	2547	A
30	f	2548	C
30	f	2549	G
30	f	2552	C
30	f	2554	A
30	f	2555	G
30	f	2561	A
30	f	2569	A
30	f	2570	U
30	f	2571	U
30	f	2572	C
30	f	2573	G
30	f	2581	U

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Mol	Chain	Res	Type
30	f	2585	G
30	f	2593	A
30	f	2594	C
30	f	2606	G
30	f	2607	G
30	f	2614	G
30	f	2648	G
30	f	2651	G
30	f	2652	U
30	f	2656	A
30	f	2674	A
30	f	2677	G
30	f	2678	A
30	f	2689	A
30	f	2691	A
30	f	2694	A
30	f	2696	A
30	f	2704	A
30	f	2714	G
30	f	2719	U
30	f	2728	G
30	f	2729	U
30	f	2740	A
30	f	2752	U
30	f	2753	G
30	f	2755	C
30	f	2772	C
30	f	2773	C
30	f	2777	G
30	f	2778	G
30	f	2788	C
30	f	2796	G
30	f	2800	G
30	f	2801	A
30	f	2803	A
30	f	2810	C
30	f	2814	G
30	f	2817	A
30	f	2818	U
30	f	2821	C
30	f	2834	G
30	f	2842	U

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Mol	Chain	Res	Type
30	f	2844	C
30	f	2845	A
30	f	2849	C
30	f	2860	U
30	f	2867	C
30	f	2871	G
30	f	2872	A
30	f	2875	U
30	f	2887	A
30	f	2898	G
30	f	2899	C
30	f	2911	A
30	f	2914	G
30	f	2923	U
30	f	2935	U
30	f	2936	A
30	f	2941	A
30	f	2942	C
30	f	2947	G
30	f	2971	A
30	f	2983	C
30	f	2990	G
30	f	2992	U
30	f	2996	U
30	f	2997	G
30	f	3006	A
30	f	3012	A
30	f	3056	U
30	f	3059	G
30	f	3078	U
30	f	3079	U
30	f	3080	G
30	f	3086	A
30	f	3092	C
30	f	3104	U
30	f	3113	A
30	f	3122	A
30	f	3130	A
30	f	3131	U
30	f	3142	A
30	f	3143	C
30	f	3151	U

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Mol	Chain	Res	Type
30	f	3154	C
30	f	3155	U
30	f	3156	U
30	f	3157	U
30	f	3165	A
30	f	3170	A
30	f	3173	G
30	f	3174	A
30	f	3175	U
30	f	3176	G
30	f	3179	U
30	f	3181	C
30	f	3186	A
30	f	3187	A
30	f	3196	U
30	f	3207	U
30	f	3209	A
30	f	3217	C
30	f	3218	A
30	f	3219	G
30	f	3228	C
30	f	3229	G
30	f	3243	A
30	f	3245	A
30	f	3247	G
30	f	3259	U
30	f	3263	G
30	f	3269	U
30	f	3270	U
30	f	3273	A
30	f	3276	G
30	f	3281	U
30	f	3287	U
30	f	3288	G
30	f	3289	G
30	f	3294	A
30	f	3295	A
30	f	3303	G
30	f	3304	U
30	f	3307	A
30	f	3313	U
30	f	3316	A

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Mol	Chain	Res	Type
30	f	3317	U
30	f	3318	G
30	f	3319	U
30	f	3320	A
30	f	3341	U
30	f	3342	A
30	f	3345	G
30	f	3351	U
30	f	3352	U
30	f	3353	G
30	f	3354	U
30	f	3355	U
30	f	3369	G
30	f	3375	A
30	f	3378	C
30	f	3382	U
30	f	3383	G
30	f	3386	G
30	f	3389	U
30	f	3390	G
30	f	3396	U
31	h	7	G
31	h	29	C
31	h	53	U
31	h	54	U
31	h	55	A
31	h	65	G
31	h	73	C
31	h	74	C
31	h	95	A
31	h	102	A
31	h	112	G
31	h	121	U
32	i	23	U
32	i	34	U
32	i	35	C
32	i	39	G
32	i	48	A
32	i	52	A
32	i	53	A
32	i	59	A
32	i	62	C

Continued on next page...

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Mol	Chain	Res	Type
32	i	63	G
32	i	80	A
32	i	81	U
32	i	82	U
32	i	83	C
32	i	84	C
32	i	85	G
32	i	86	U
32	i	87	G
32	i	90	U
32	i	95	G
32	i	104	A
32	i	105	A
32	i	106	C
32	i	111	A
32	i	113	U
32	i	125	U
32	i	126	A
32	i	138	A
32	i	151	C
32	i	152	G
32	i	157	U
32	i	158	U
49	x	5	G
49	x	9	G
49	x	15	G
49	x	16	U
49	x	17	C
49	x	18	G
49	x	22	G
49	x	28	U
49	x	33	U
49	x	37	A
49	x	38	U
49	x	39	G
49	x	46	G
49	x	48	C
49	x	56	C
49	x	57	G
49	x	58	A
49	x	60	U
49	x	74	C

Continued on next page...

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Mol	Chain	Res	Type
49	y	7	G
49	y	9	G
49	y	13	U
49	y	17	C
49	y	23	C
49	y	26	G
49	y	36	C
49	y	38	U
49	y	43	G
49	y	45	G
49	y	46	G
49	y	47	U
49	y	48	C
49	y	56	C
49	y	58	A
49	y	61	C
49	y	75	C
49	y	76	A

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
47	5CT	v	51	47	13,14,15	0.79	0	8,15,17	1.30	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	5CT	v	51	47	-	9/13/14/16	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	v	51	5CT	C4-C3-C2	-2.21	108.81	113.47

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
47	v	51	5CT	NZ-C1-C2-C3
47	v	51	5CT	O1-C2-C3-C4
47	v	51	5CT	C2-C3-C4-N1
47	v	51	5CT	C-CA-CB-CG
47	v	51	5CT	N-CA-CB-CG
47	v	51	5CT	NZ-C1-C2-O1
47	v	51	5CT	C1-C2-C3-C4
47	v	51	5CT	C2-C1-NZ-CE
47	v	51	5CT	CE-CD-CG-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	v	51	5CT	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 20 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
55	SPD	f	3401	-	9,9,9	0.32	0	8,8,8	0.85	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	SPD	f	3401	-	-	5/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	f	3401	SPD	C3-C4-C5-N6
55	f	3401	SPD	N6-C7-C8-C9
55	f	3401	SPD	C2-C3-C4-C5
55	f	3401	SPD	C4-C5-N6-C7
55	f	3401	SPD	C8-C7-N6-C5

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	f	3401	SPD	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

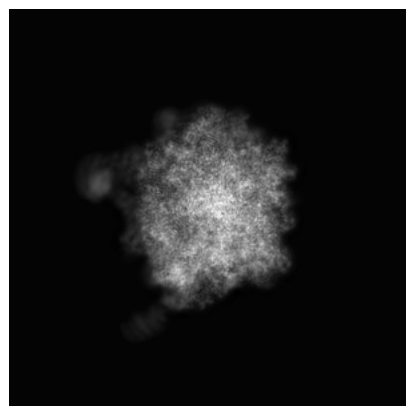
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15427. These allow visual inspection of the internal detail of the map and identification of artifacts.

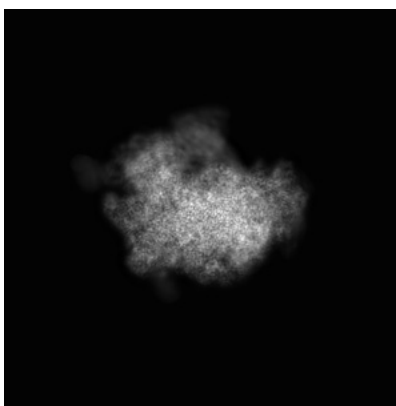
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

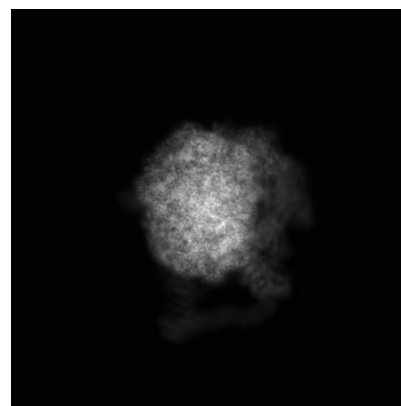
6.1.1 Primary map



X

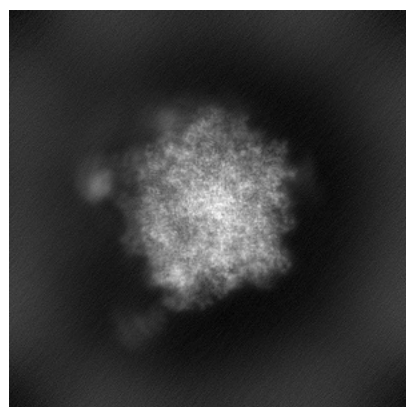


Y

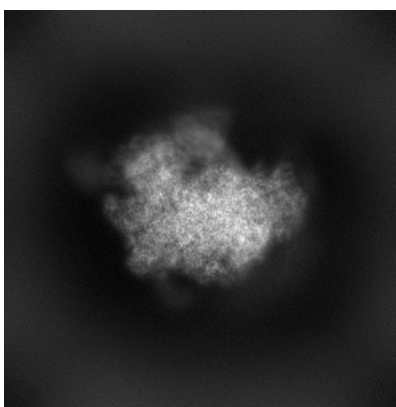


Z

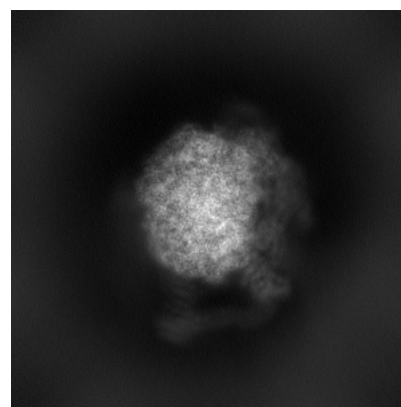
6.1.2 Raw map



X



Y

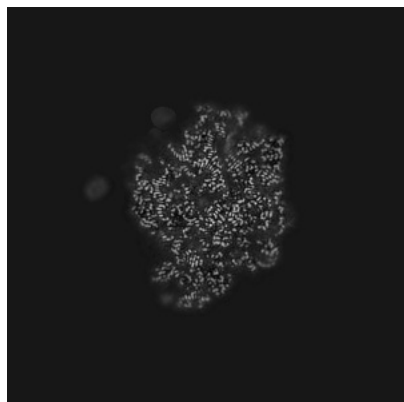


Z

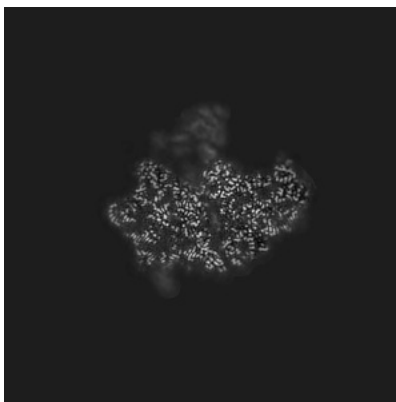
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

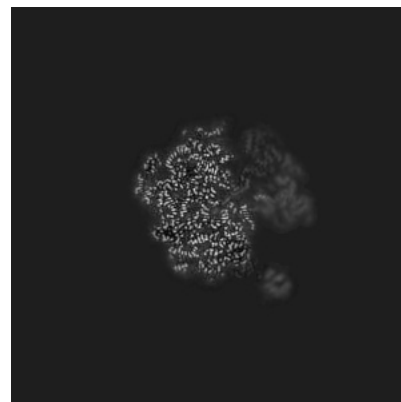
6.2.1 Primary map



X Index: 225

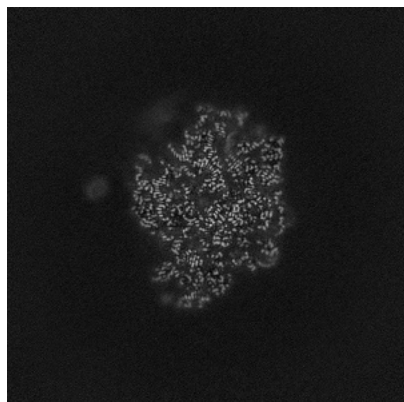


Y Index: 225

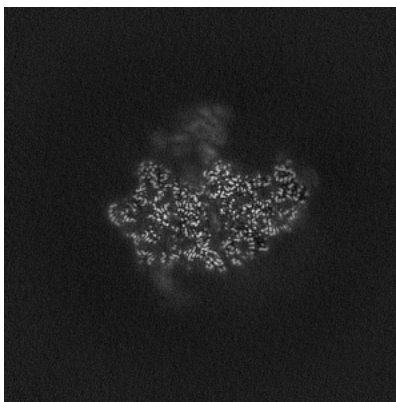


Z Index: 225

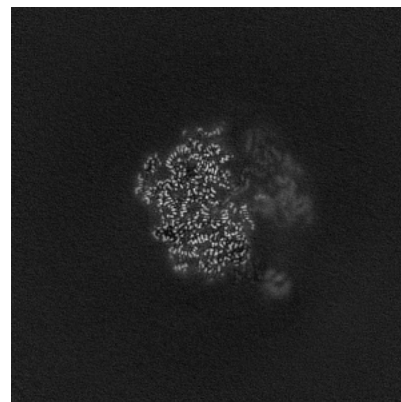
6.2.2 Raw map



X Index: 225



Y Index: 225

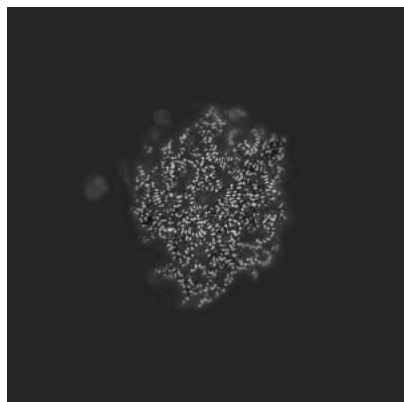


Z Index: 225

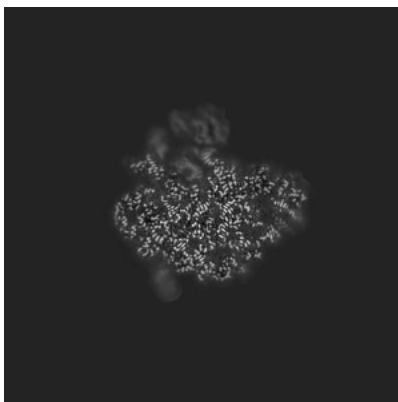
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

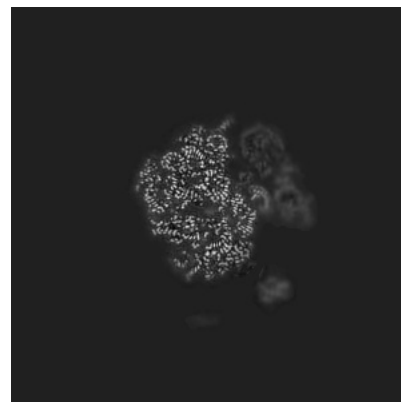
6.3.1 Primary map



X Index: 219

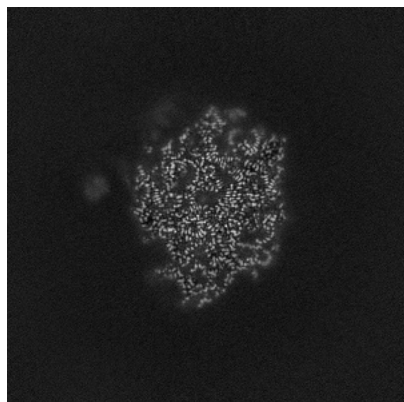


Y Index: 237

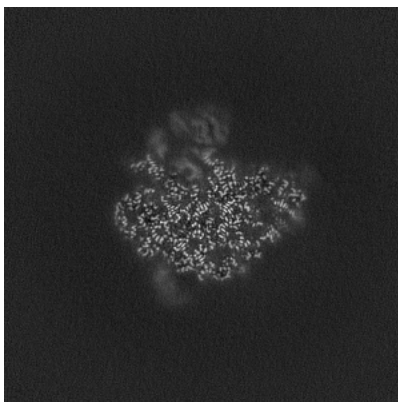


Z Index: 231

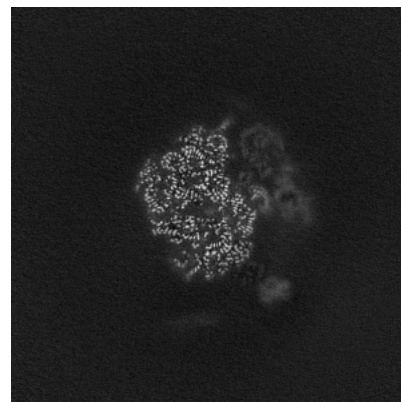
6.3.2 Raw map



X Index: 219



Y Index: 237

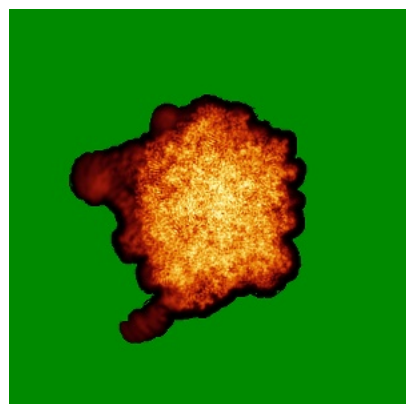


Z Index: 231

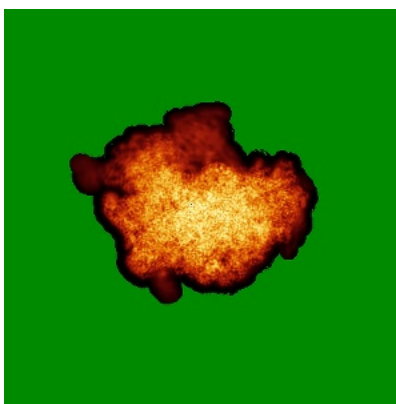
The images above show the largest variance slices of the map in three orthogonal directions.

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

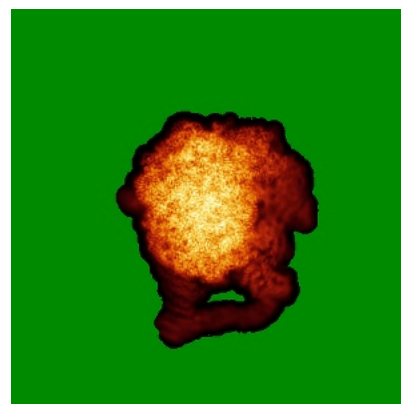
6.4.1 Primary map



X

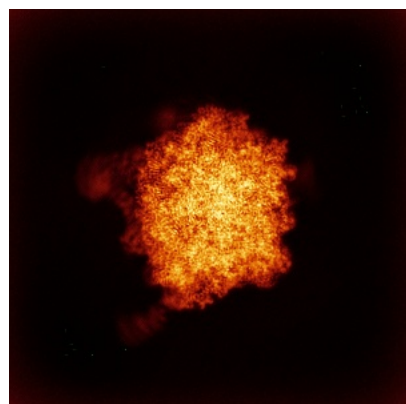


Y

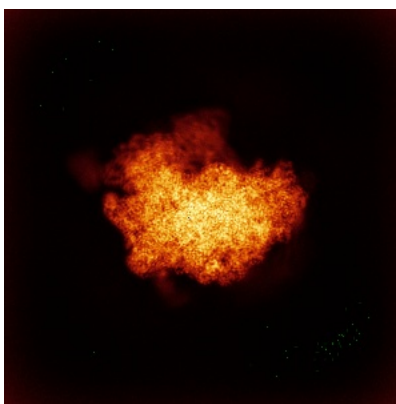


Z

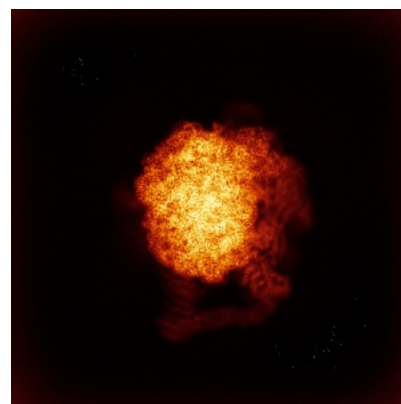
6.4.2 Raw map



X



Y

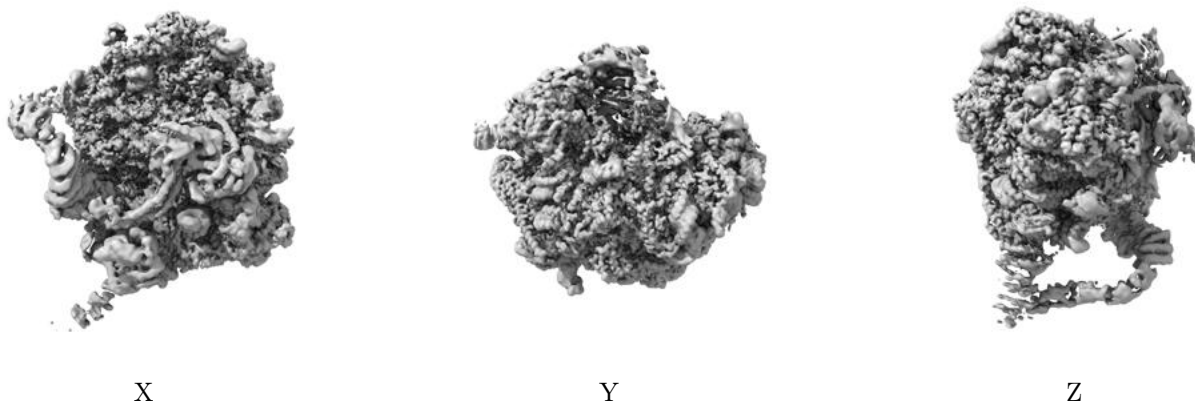


Z

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

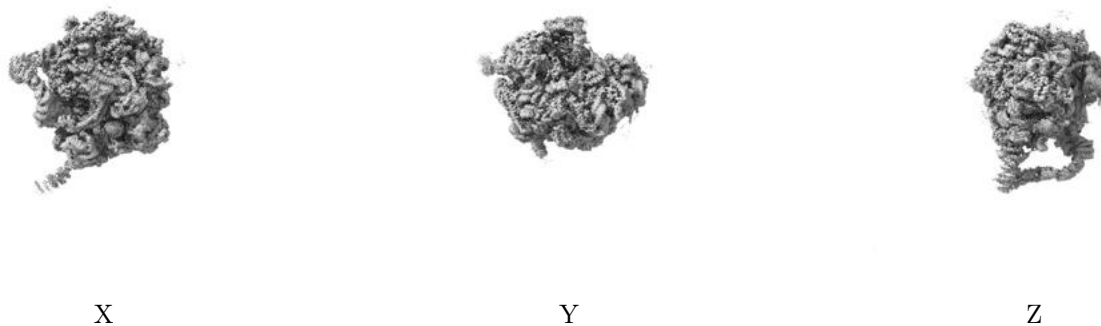
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

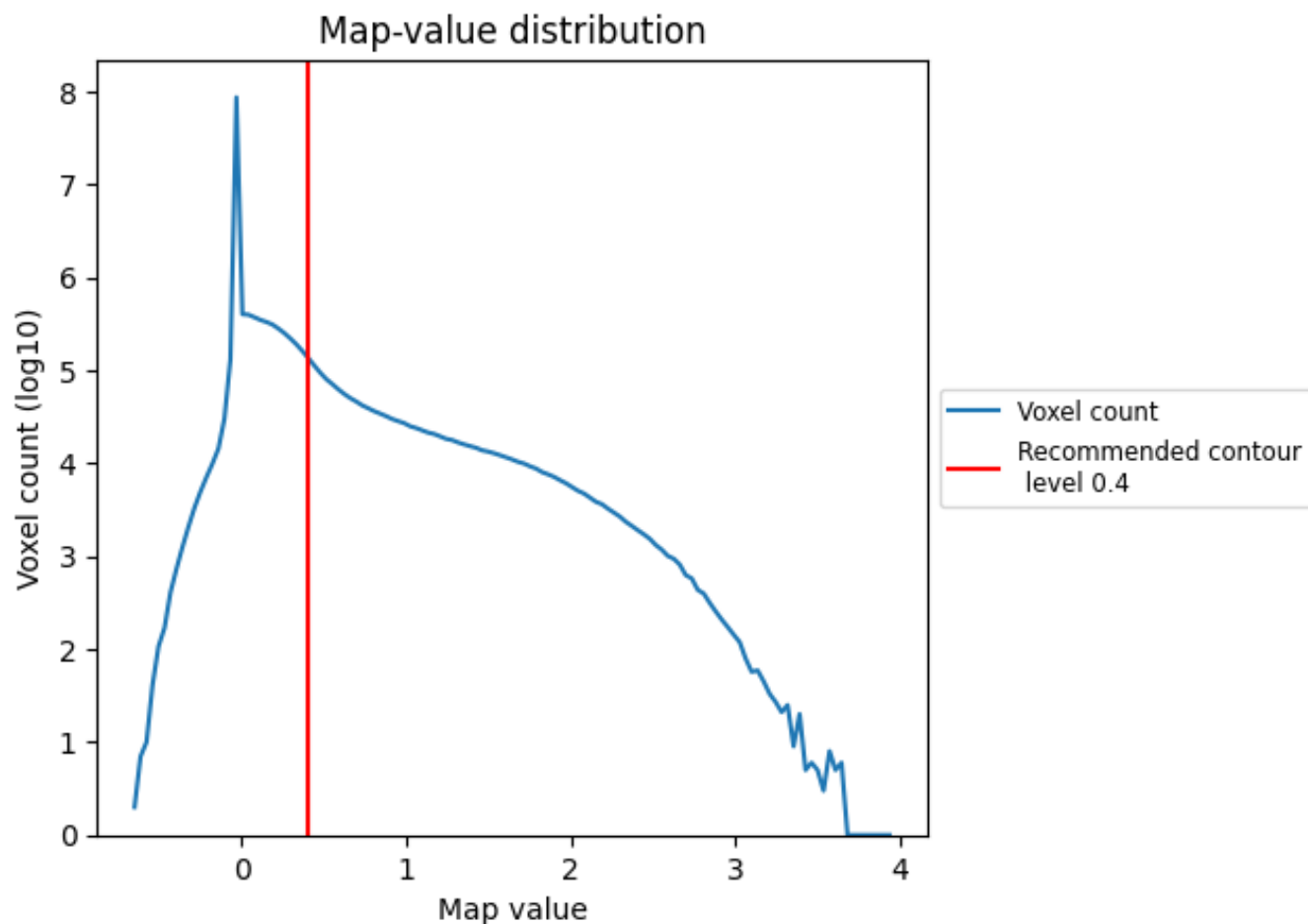
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

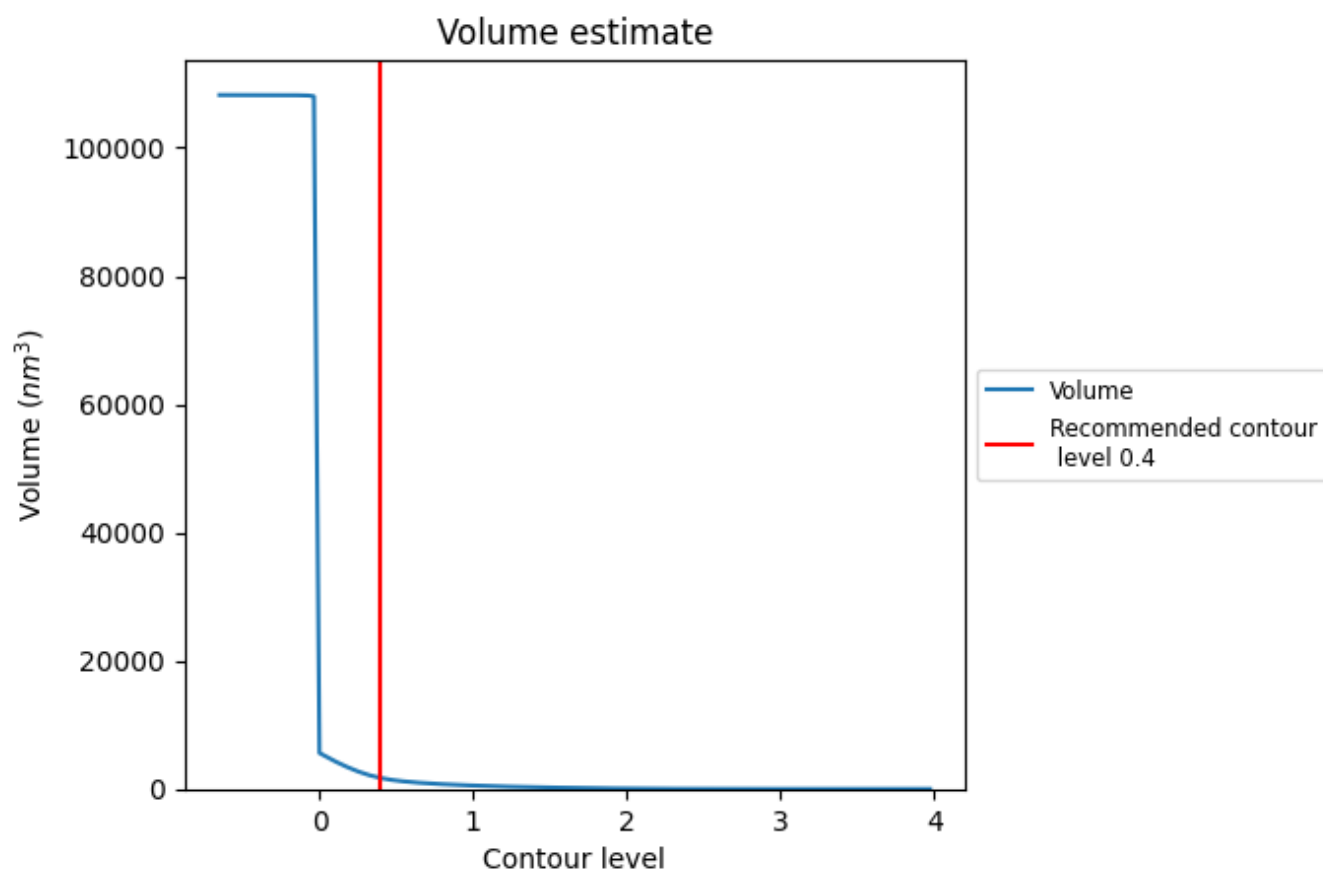
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

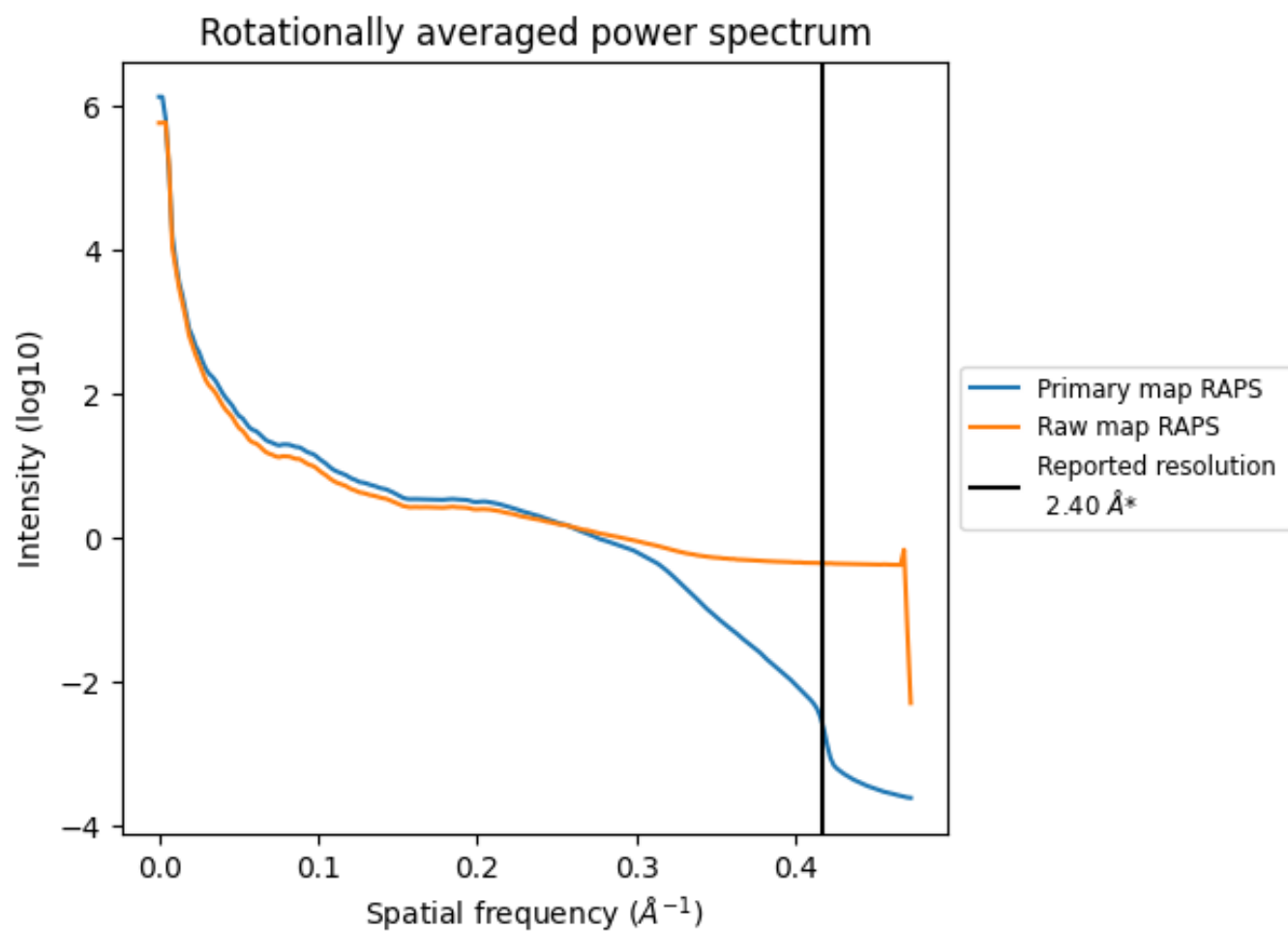
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1709 nm^3 ; this corresponds to an approximate mass of 1544 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 ⓘ

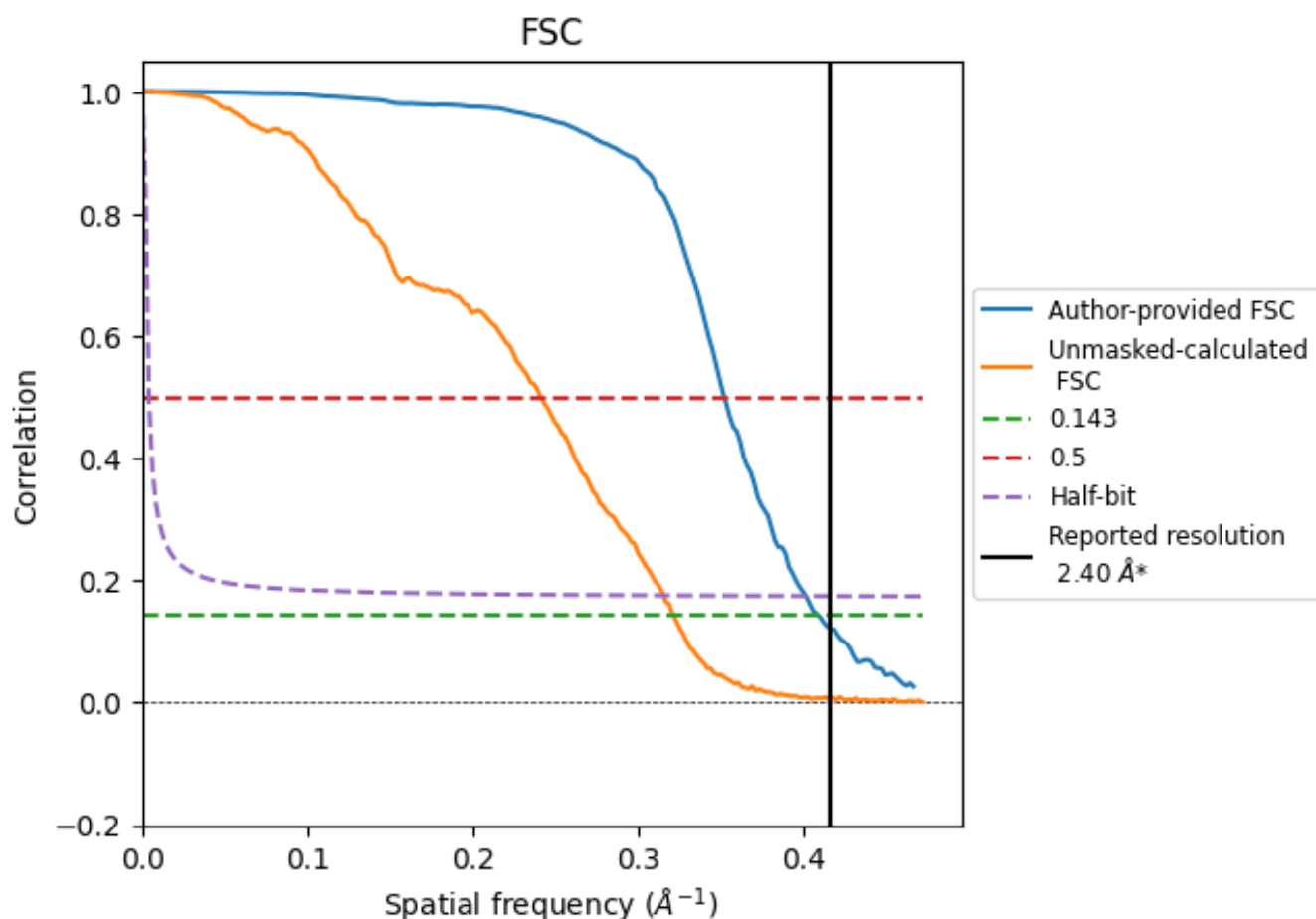


*Reported resolution corresponds to spatial frequency of 0.417 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.417 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

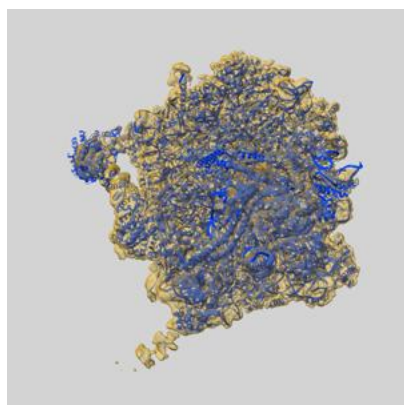
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.44	2.84	2.49
Unmasked-calculated*	3.11	4.14	3.17

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.11 differs from the reported value 2.4 by more than 10 %

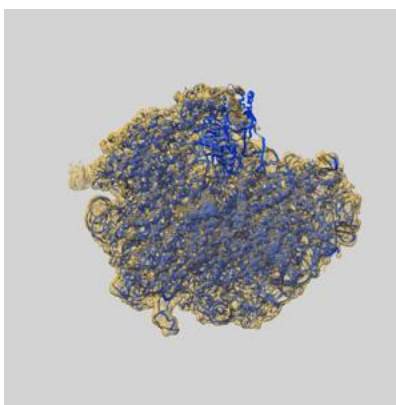
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15427 and PDB model 8AGX. Per-residue inclusion information can be found in section [3](#) on page [15](#).

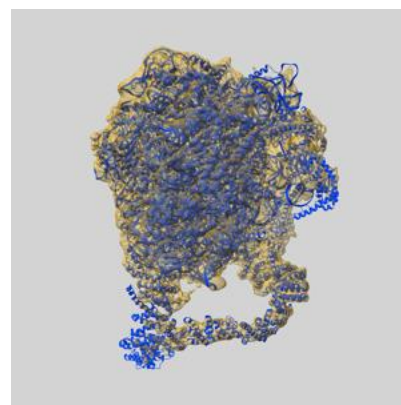
9.1 Map-model overlay [i](#)



X



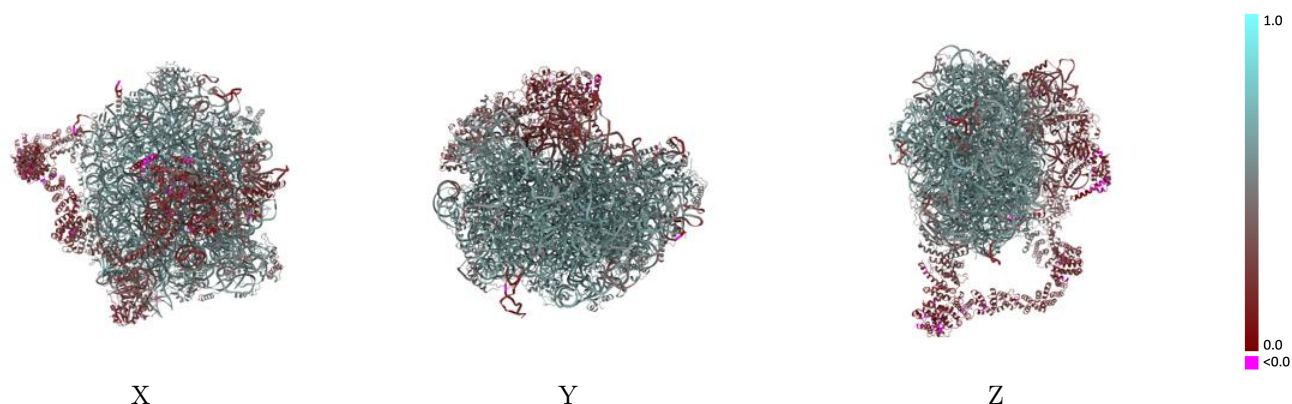
Y



Z

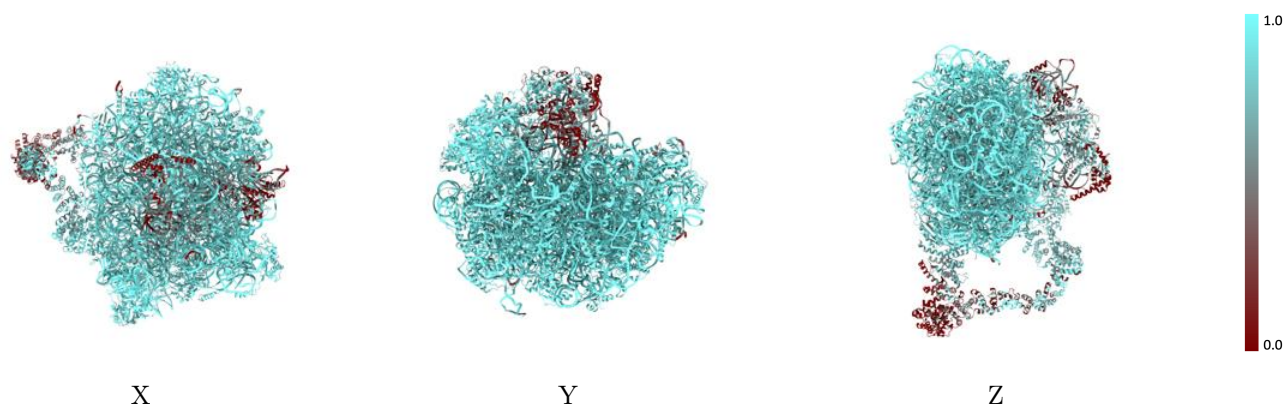
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



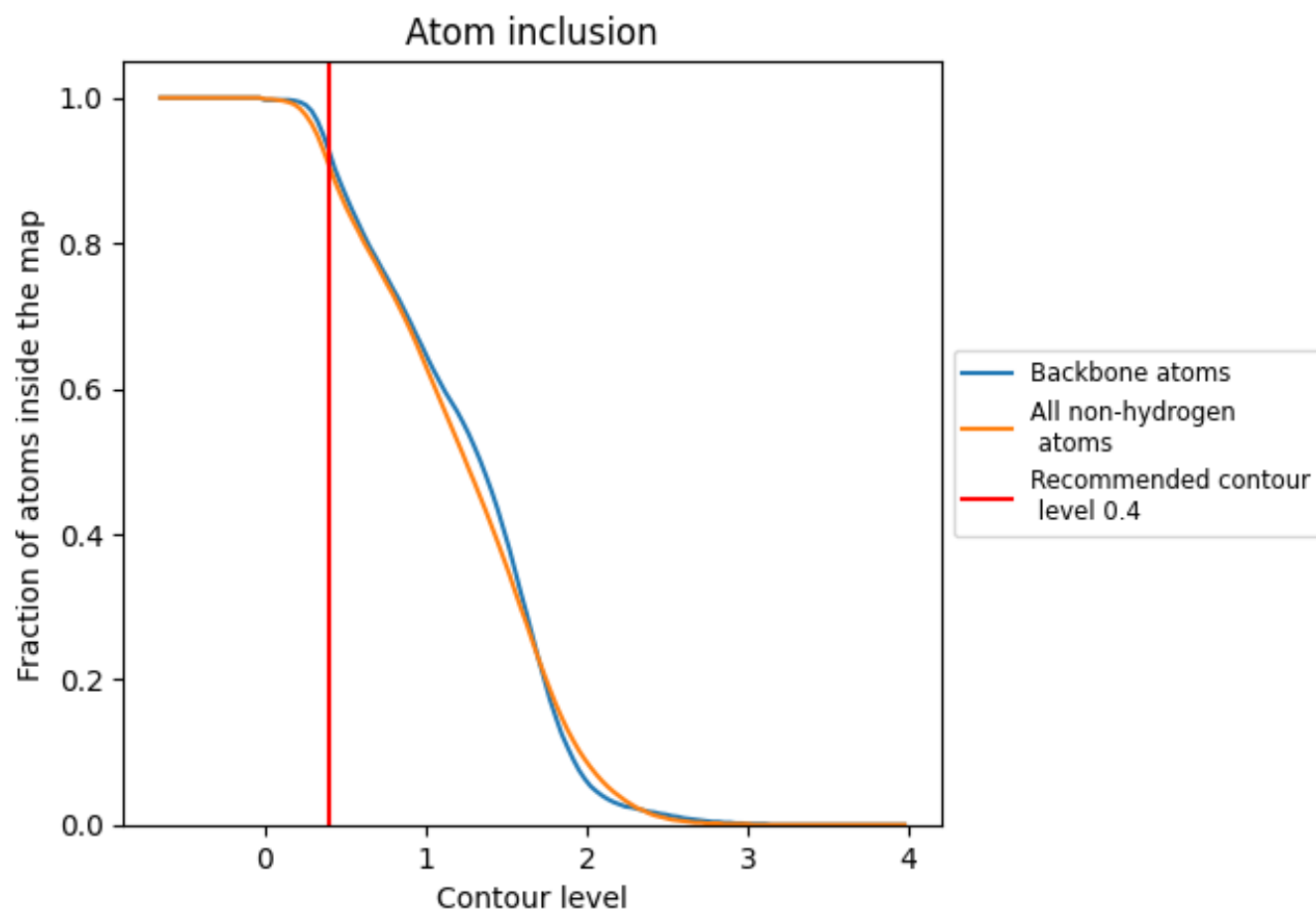
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 91% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9060	 0.5200
0	 0.8400	 0.2790
1	 0.9890	 0.4180
A	 0.9910	 0.6220
B	 0.9800	 0.5990
C	 0.9710	 0.5960
D	 0.9800	 0.5970
E	 0.9380	 0.5600
F	 0.9790	 0.5880
G	 0.9690	 0.5770
H	 0.9180	 0.4740
I	 0.9670	 0.5830
J	 0.9600	 0.5800
K	 0.9710	 0.5860
L	 0.9760	 0.5810
M	 0.9520	 0.5350
N	 0.9820	 0.6050
O	 0.9560	 0.5510
P	 0.9390	 0.5370
Q	 0.9390	 0.5670
R	 0.9840	 0.6140
S	 0.9920	 0.6230
T	 0.9680	 0.5850
U	 0.9680	 0.5700
V	 0.9570	 0.5380
W	 1.0000	 0.6370
X	 0.9200	 0.5010
Y	 0.9980	 0.6160
Z	 0.9650	 0.5800
a	 0.6040	 0.2130
b	 0.9600	 0.5860
c	 0.9720	 0.5850
d	 0.7710	 0.4410
e	 0.5430	 0.2490
f	 0.9830	 0.5790



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Chain	Atom inclusion	Q-score
h	 0.9990	 0.5830
i	 0.9950	 0.6070
j	 0.9880	 0.6160
k	 0.9790	 0.5960
l	 0.9750	 0.5890
m	 0.9410	 0.5020
n	 0.9530	 0.5390
o	 0.9740	 0.5840
p	 0.9520	 0.5350
q	 0.9600	 0.5600
r	 0.9580	 0.5560
s	 0.9360	 0.4690
t	 0.9720	 0.5750
u	 0.9720	 0.5610
v	 0.4730	 0.3880
w	 0.1540	 0.2370
x	 0.4690	 0.2580
y	 0.8790	 0.2370
z	 0.9150	 0.2820