



## Full wwPDB EM Validation Report ⓘ

Apr 6, 2026 – 01:01 AM UTC

PDB ID : 9EVT / pdb\_00009evt  
EMDB ID : EMD-50014  
Title : Structure of the small subunit of the flowering plant mitoribosome with the maturation factor RsgA  
Authors : Waltz, F.; Skaltsogiannis, V.; Giege, P.  
Deposited on : 2024-04-02  
Resolution : 2.27 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

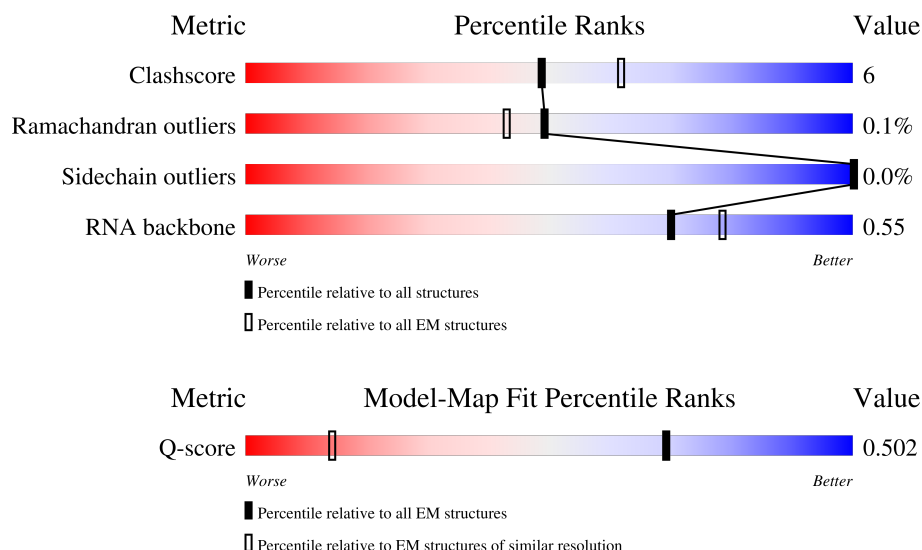
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.27 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.





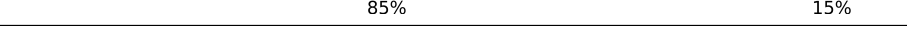




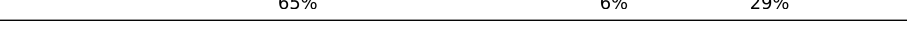



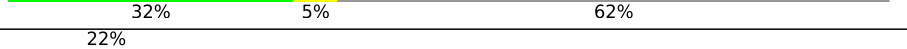




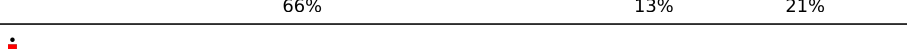

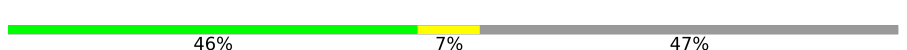





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	3593 ( 1.77 - 2.77 )

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  $\geq 3$ , 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	212	
2	B	554	
3	C	362	

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Mol	Chain	Length	Quality of chain
4	D	501	
5	E	138	
6	F	157	
7	G	129	
8	H	383	
9	I	228	
10	J	304	
11	K	125	
12	L	154	
13	M	155	
14	N	414	
15	O	136	
16	P	110	
17	Q	237	
18	R	212	
19	S	100	
20	T	94	
21	U	192	
22	V	193	
23	W	483	
24	X	496	
25	Y	102	
26	Z	153	
27	7	496	
28	a	424	

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Mol	Chain	Length	Quality of chain
29	b	80	
30	c	128	
31	d	110	
32	e	383	
33	f	410	
34	h	384	
35	i	725	
36	k	153	
37	2	1560	

## 2 Entry composition [i](#)

There are 42 unique types of molecules in this entry. The entry contains 85715 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 Ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	204	Total	C	N	O	S	0	0
			1611	1032	284	285	10		

- Molecule 2 is a protein called Small ribosomal subunit protein uS3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	467	Total	C	N	O	S	0	0
			3877	2520	701	643	13		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	22	TRP	ARG	conflict	UNP A0A068BCX1
B	172	LEU	SER	conflict	UNP A0A068BCX1
B	202	LYS	ARG	conflict	UNP A0A068BCX1
B	296	LEU	SER	conflict	UNP A0A068BCX1
B	512	CYS	ARG	conflict	UNP A0A068BCX1
B	524	VAL	ALA	conflict	UNP A0A068BCX1
B	533	LEU	SER	conflict	UNP A0A068BCX1

- Molecule 3 is a protein called Ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	333	Total	C	N	O	S	0	0
			2806	1793	540	462	11		

- Molecule 4 is a protein called S5 DRBM domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	417	Total	C	N	O	S	0	0
			3425	2146	603	664	12		

- Molecule 5 is a protein called bS6m.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	101	Total	C	N	O	S	0	0
			823	535	145	138	5		

- Molecule 6 is a protein called uS7m,Small ribosomal subunit protein uS7m,Small ribosomal subunit protein uS7m.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	157	Total	C	N	O	S	0	0
			1254	793	244	213	4		

- Molecule 7 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	128	Total	C	N	O	S	0	0
			1037	652	193	189	3		

- Molecule 8 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	211	Total	C	N	O	S	0	0
			1662	1042	306	309	5		

- Molecule 9 is a protein called Small ribosomal subunit protein uS10 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	113	Total	C	N	O	S	0	0
			941	602	174	159	6		

- Molecule 10 is a protein called Ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	127	Total	C	N	O	S	0	0
			993	612	196	181	4		

- Molecule 11 is a protein called Small ribosomal subunit protein uS12m.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	124	Total	C	N	O	S	0	0
			992	614	209	165	4		

- Molecule 12 is a protein called uS13m.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	109	Total	C	N	O	S	0	0
			864	523	183	153	5		

- Molecule 13 is a protein called Small ribosomal subunit protein uS14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	101	Total	C	N	O	S	0	0
			843	524	174	140	5		

- Molecule 14 is a protein called Small ribosomal subunit protein uS15c.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	116	Total	C	N	O	S	0	0
			941	593	170	171	7		

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	110	Total	C	N	O	S	0	0
			869	550	169	144	6		

- Molecule 16 is a protein called Small ribosomal subunit protein uS17c.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	91	Total	C	N	O	S	0	0
			717	455	135	124	3		

- Molecule 17 is a protein called Small ribosomal subunit protein bS18c.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	90	Total	C	N	O	S	0	0
			724	460	127	134	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	250	ILE	VAL	conflict	UNP A0A078FCZ9

- Molecule 18 is a protein called Small ribosomal subunit protein uS19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	166	Total	C	N	O	S	0	0
			1299	819	236	237	7		

- Molecule 19 is a protein called Ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	75	Total	C	N	O	S	0	0
			611	386	120	103	2		

- Molecule 20 is a protein called 30S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	50	Total	C	N	O	S	0	0
			408	260	79	68	1		

- Molecule 21 is a protein called Small ribosomal subunit protein mS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	127	Total	C	N	O	S	0	0
			1016	647	185	179	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	81	GLN	PRO	conflict	UNP A0A3P6DYP2

- Molecule 22 is a protein called mS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	164	Total	C	N	O	S	0	0
			1399	874	266	255	4		

- Molecule 23 is a protein called Small ribosomal subunit protein mS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	380	Total	C	N	O	S	0	0
			3062	1955	535	559	13		

- Molecule 24 is a protein called BnaC06g06470D protein.



Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	204	Total	C	N	O	S	0	0
			1613	1011	262	329	11		

- Molecule 25 is a protein called MOSC domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	98	Total	C	N	O	S	0	0
			793	495	159	137	2		

- Molecule 26 is a protein called Mitochondrial 28S ribosomal protein S34.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	81	Total	C	N	O	S	0	0
			660	428	125	105	2		

- Molecule 27 is a protein called EngC GTPase domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	7	363	Total	C	N	O	S	0	0
			2878	1824	514	526	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
7	385	MET	GLN	conflict	UNP A0A0D3CYN0

- Molecule 28 is a protein called Small ribosomal subunit protein mS35 mitochondrial conserved domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	a	315	Total	C	N	O	S	0	0
			2486	1546	448	482	10		

- Molecule 29 is a protein called IMS import disulfide relay-system CHCH-CHCH-like Cx9C domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	b	73	Total	C	N	O	S	0	0
			581	361	108	104	8		

- Molecule 30 is a protein called Small ribosomal subunit protein mS38.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	c	26	Total	C	N	O	S	0	0
			232	145	54	32	1		

- Molecule 31 is a protein called IGR domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	d	78	Total	C	N	O	S	0	0
			616	403	110	102	1		

- Molecule 32 is a protein called mS45.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	e	246	Total	C	N	O	S	0	0
			2074	1310	374	380	10		

- Molecule 33 is a protein called mS47.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	f	375	Total	C	N	O	S	0	0
			2898	1825	484	569	20		

- Molecule 34 is a protein called (rape) hypothetical protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	h	310	Total	C	N	O	S	0	0
			2463	1557	438	455	13		

- Molecule 35 is a protein called PROP1-like PPR domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	i	306	Total	C	N	O	S	0	0
			2487	1567	419	487	14		

- Molecule 36 is a protein called RRM domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	22	Total	C	N	O	S	0	0
			177	113	34	27	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	9	ARG	LYS	conflict	UNP A0A3P6FEP3
k	15	LYS	ARG	conflict	UNP A0A3P6FEP3

- Molecule 37 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	2	1560	Total	C	N	O	P	0	0
			33424	14925	6097	10842	1560		

- Molecule 38 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
38	K	1	Total	K	0
			1	1	
38	2	9	Total	K	0
			9	9	

- Molecule 39 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
39	T	1	Total	Mg	0
			1	1	
39	W	1	Total	Mg	0
			1	1	
39	7	1	Total	Mg	0
			1	1	
39	2	82	Total	Mg	0
			82	82	

- Molecule 40 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).




Mol	Chain	Residues	Atoms					AltConf
42	7	1	Total	C	N	O	P	0
			32	10	5	14	3	

### 3 Residue-property plots

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

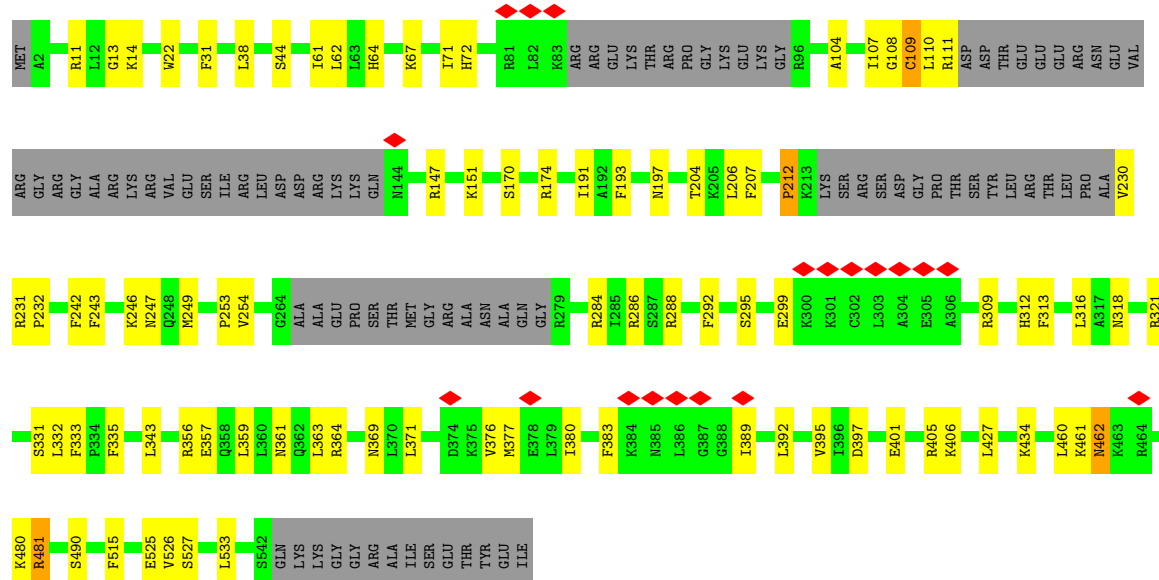
#### • Molecule 1: Ribosomal protein S2

Chain A: 




#### • Molecule 2: Small ribosomal subunit protein uS3m

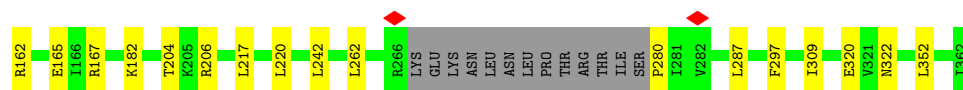
Chain B: 



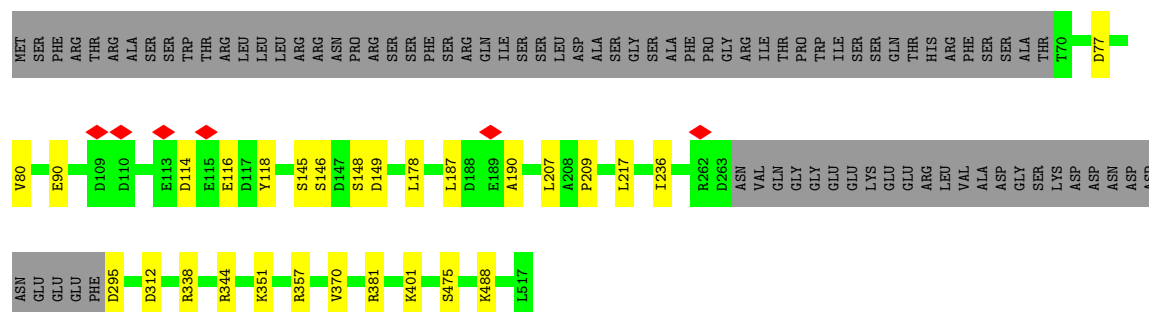
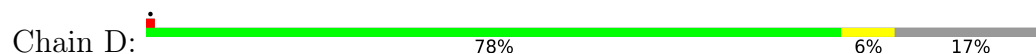
#### • Molecule 3: Ribosomal protein S4

Chain C: 

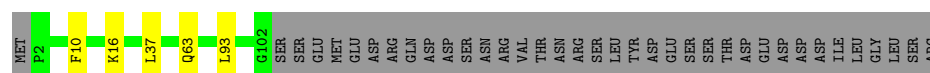




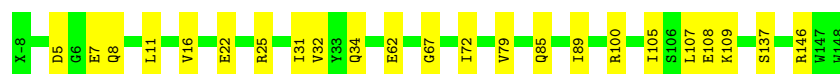
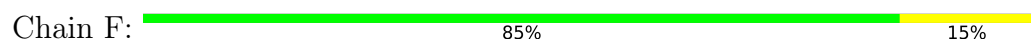
- Molecule 4: S5 DRBM domain-containing protein



- Molecule 5: bS6m



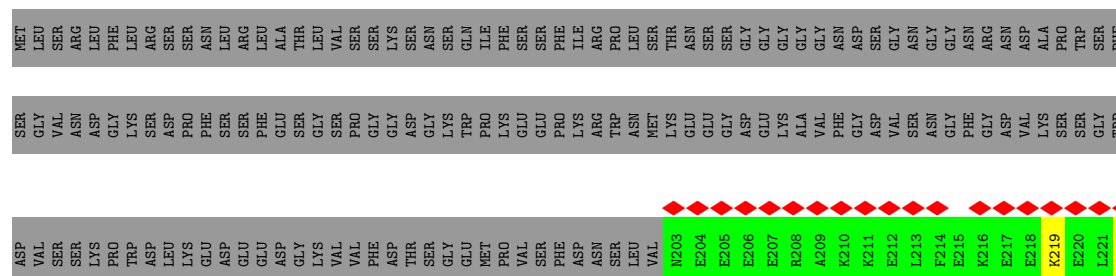
- Molecule 6: uS7m, Small ribosomal subunit protein uS7m, Small ribosomal subunit protein uS7m



- Molecule 7: 40S ribosomal protein S15a



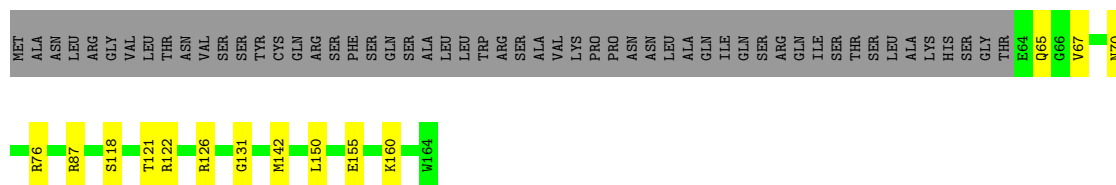
- Molecule 8: 30S ribosomal protein S9







Chain M:  56% 9% 35%



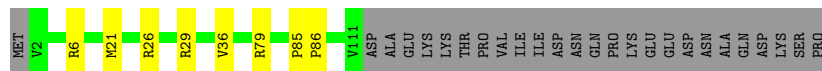
• Molecule 14: Small ribosomal subunit protein uS15c

Chain N:  27% 72%



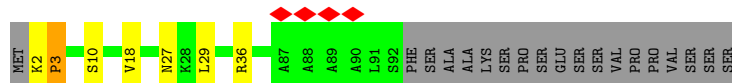
• Molecule 15: 30S ribosomal protein S16

Chain O:  75% 6% 19%



• Molecule 16: Small ribosomal subunit protein uS17c

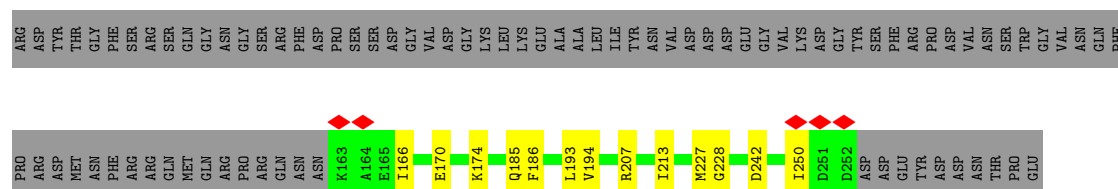
Chain P:  76% 5% 17%



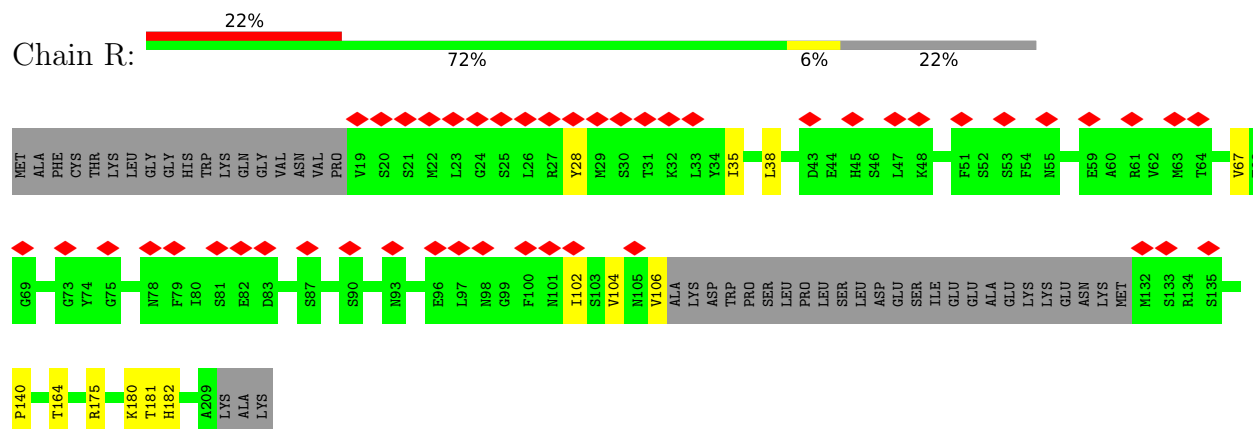
• Molecule 17: Small ribosomal subunit protein bS18c

Chain Q:  32% 5% 62%

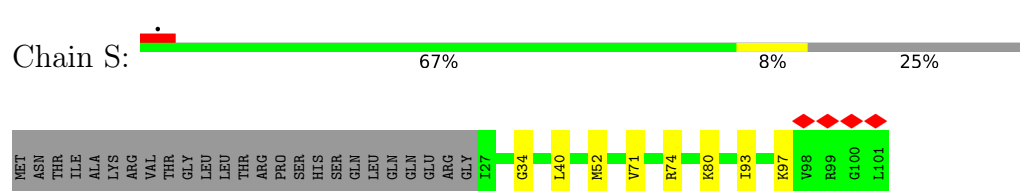




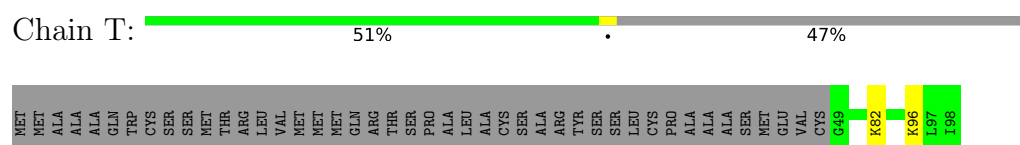
- Molecule 18: Small ribosomal subunit protein uS19m



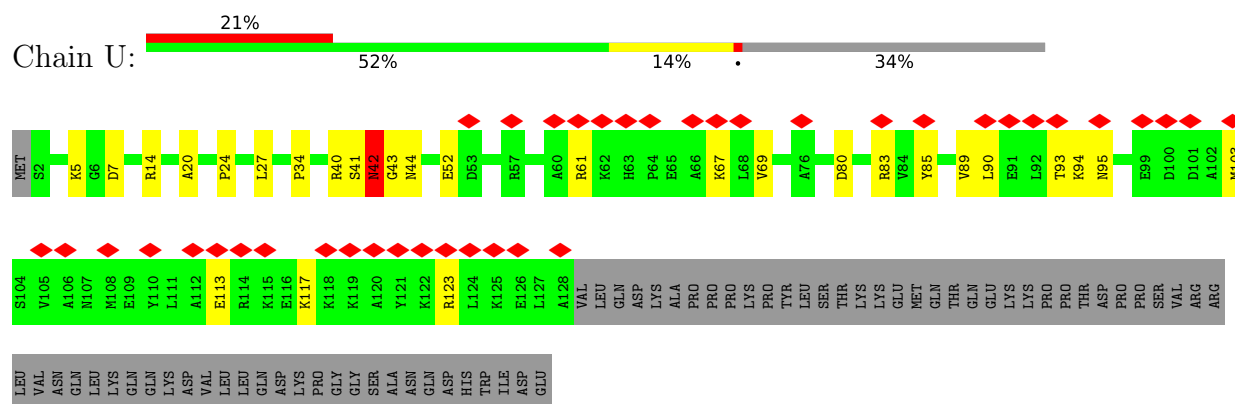
- Molecule 19: Ribosomal protein S21



- Molecule 20: 30S ribosomal protein S31, mitochondrial



- Molecule 21: Small ribosomal subunit protein mS23



- Molecule 22: mS26

Sequence logo for the 10th position. The y-axis represents information content in bits, ranging from 0 to 0.4. The x-axis shows the amino acid sequence from MET to L155. The sequence is: MET, SER, LEU, CYS, ASN, GLN, LEU, SER, ARG, LEU, VAL, LYS, GLN, SER, PRO, THR, LYS, GLN, SER, LEU, ARG, SER, PHE, SER, SER, ALA, ALA, T32, H36, E39, T40, E47, S48, Y49, E89, R92, R113, R114, K117, A118, A119, A120, A121, K122, V123, R124, E142, L155. The sequence is color-coded: MET (grey), SER (grey), LEU (grey), CYS (grey), ASN (grey), GLN (grey), LEU (grey), SER (grey), ARG (grey), LEU (grey), VAL (grey), LYS (grey), GLN (grey), SER (grey), PRO (grey), THR (grey), LYS (grey), GLN (grey), SER (grey), LEU (grey), ARG (grey), SER (grey), PHE (grey), SER (grey), SER (grey), ALA (grey), ALA (grey), T32 (red), H36 (yellow), E39 (yellow), T40 (yellow), E47 (yellow), S48 (green), Y49 (green), E89 (yellow), R92 (yellow), R113 (yellow), R114 (yellow), K117 (yellow), A118 (green), A119 (green), A120 (green), A121 (green), K122 (green), V123 (green), R124 (yellow), E142 (yellow), L155 (yellow). The sequence is aligned with a reference sequence: E159, I176, K184, E187, A188, L189, S192, L195. The reference sequence is color-coded: E159 (yellow), I176 (yellow), K184 (yellow), E187 (yellow), A188 (green), L189 (yellow), S192 (yellow), L195 (green). A red diamond is positioned above the L195 residue.

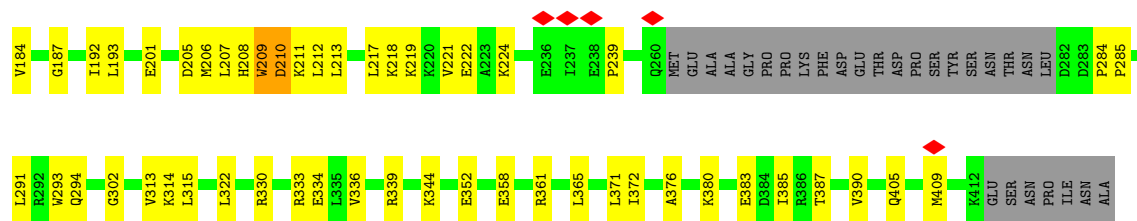
- Chain W:  66% 13% 21%

[illegible]

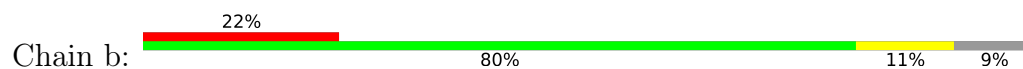
- Chain X:  33% 8% 59%

[illegible]

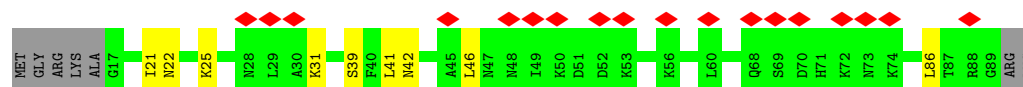
- |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |      |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| PRO | PRO | PRO | GLU | SER | SER | SER | PRO | PRO | ILE | GLU | SER | SER | ASN | LYS | ASP | LEU | ALA | VAL | GLU | ASP | V77 | G78 | F90 | N91 | E92 | G93 | N94 | I102 | E103 | A104 | L105 | R108 | T117 | D118 | V121 | M122 | D123 | S124 | L125 | Q126 | M127 | Q128 | D151 | D155 | E177 | K178 | K179 | W180 | D181 | V182 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|



- Molecule 29: IMS import disulfide relay-system CHCH-CHCH-like Cx9C domain-containing protein



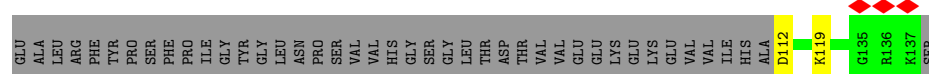
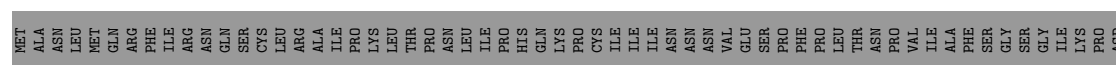
Chain b:



- Molecule 30: Small ribosomal subunit protein mS38



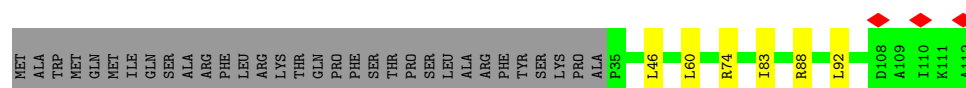
Chain c:



- Molecule 31: IGR domain-containing protein



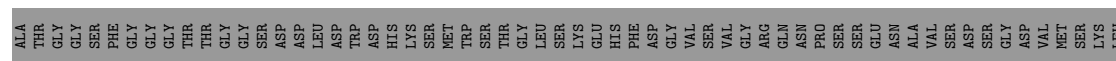
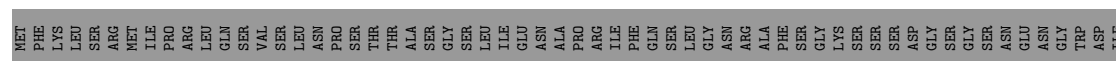
Chain d:



- Molecule 32: mS45



Chain e:

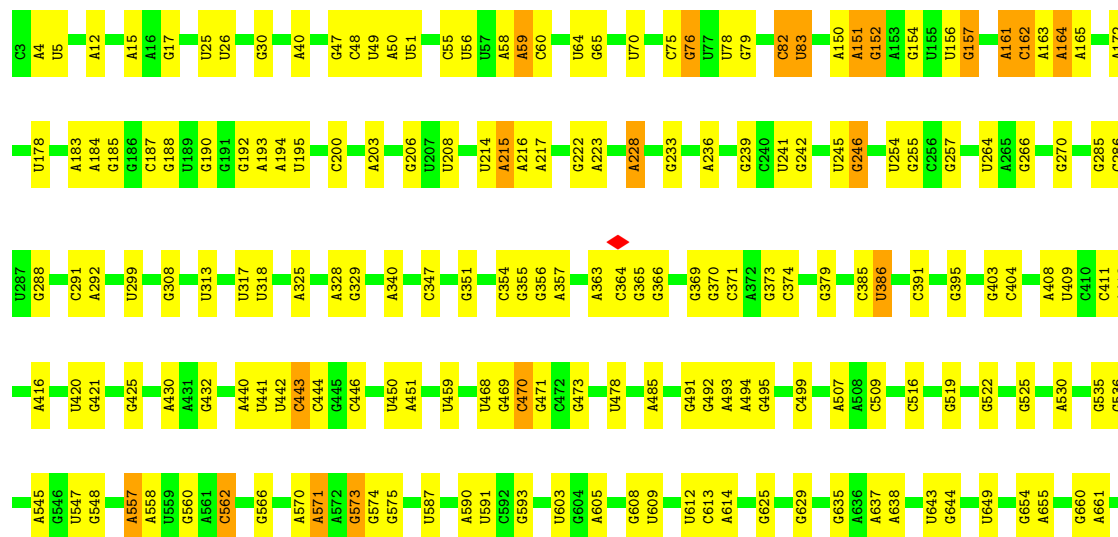


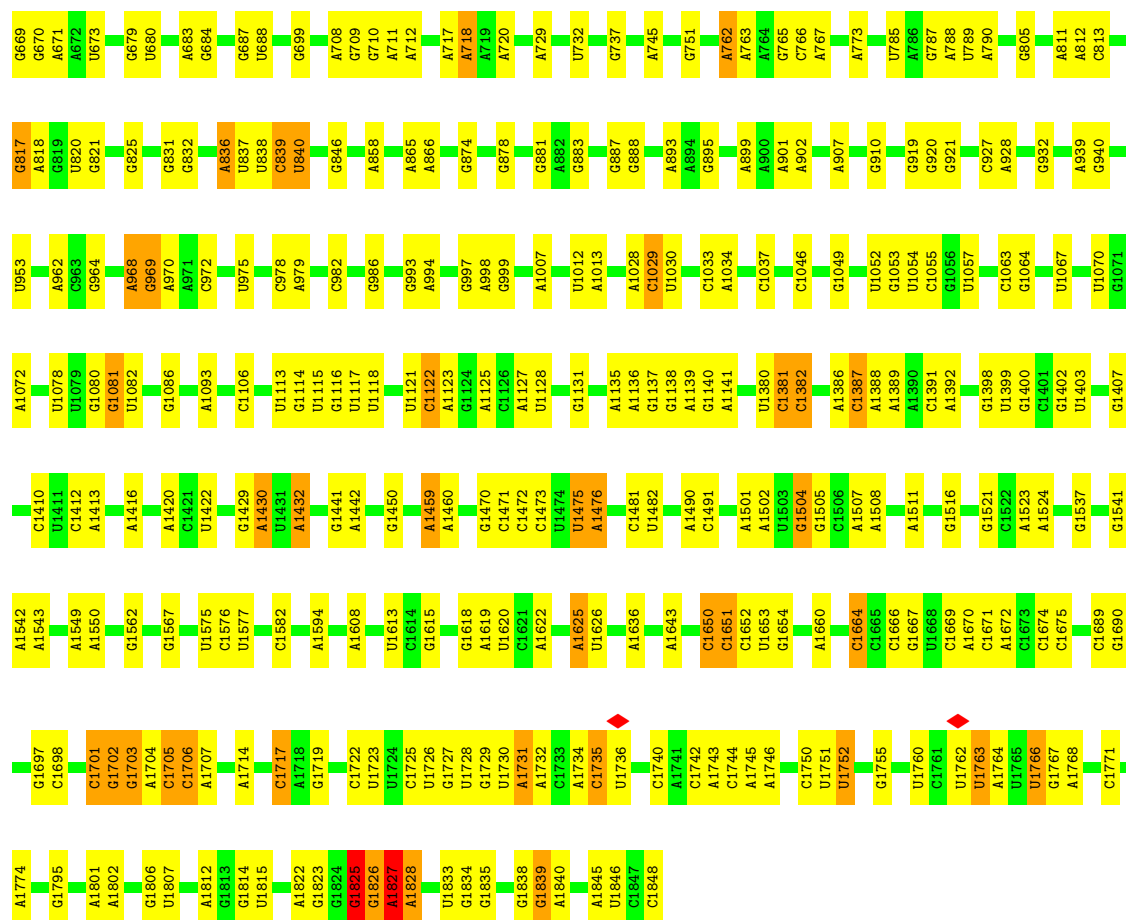
- Molecule 33: mS47



Chain f:









## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	208855	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50.96	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	165000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	1.059	Depositor
Minimum map value	-0.572	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.0377	Depositor
Map size ( $\text{\AA}$ )	524.87823, 524.87823, 524.87823	wwPDB
Map dimensions	588, 588, 588	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.89265007, 0.89265007, 0.89265007	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, 2MG, GTP, MG, K, MA6, UR3, G7M, 4OC, ATP

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	0.12	0/1647	0.34	0/2227
2	B	0.23	0/3969	0.50	1/5320 (0.0%)
3	C	0.15	0/2859	0.38	1/3828 (0.0%)
4	D	0.15	0/3474	0.38	0/4647
5	E	0.11	0/838	0.32	0/1121
6	F	0.16	0/1225	0.42	0/1641
7	G	0.15	0/1054	0.36	0/1418
8	H	0.20	0/1687	0.49	0/2262
9	I	0.19	0/964	0.43	0/1293
10	J	0.12	0/1005	0.34	0/1346
11	K	0.14	0/1009	0.36	0/1345
12	L	0.14	0/874	0.36	0/1165
13	M	0.17	0/856	0.38	0/1134
14	N	0.13	0/958	0.34	0/1280
15	O	0.16	0/890	0.37	0/1196
16	P	0.17	0/730	0.44	1/984 (0.1%)
17	Q	0.12	0/733	0.32	0/978
18	R	0.17	0/1323	0.37	0/1772
19	S	0.15	0/614	0.33	0/809
20	T	0.16	0/416	0.37	0/547
21	U	0.39	2/1037 (0.2%)	0.55	1/1395 (0.1%)
22	V	0.21	0/1423	0.33	0/1895
23	W	0.17	0/3139	0.40	0/4250
24	X	0.22	0/1644	0.46	0/2216
25	Y	0.42	0/807	0.50	0/1077
26	Z	0.12	0/680	0.34	0/914
27	7	0.18	0/2930	0.45	0/3952
28	a	0.28	0/2523	0.60	5/3386 (0.1%)
29	b	0.19	0/589	0.54	0/785
30	c	0.11	0/233	0.27	0/296
31	d	0.16	0/628	0.33	0/840
32	e	0.15	0/2118	0.38	0/2828

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	f	0.17	0/2955	0.40	1/3999 (0.0%)
34	h	0.18	0/2511	0.44	0/3391
35	i	0.14	0/2532	0.36	0/3400
36	k	0.07	0/181	0.21	0/239
37	2	0.21	2/37258 (0.0%)	0.34	2/58090 (0.0%)
All	All	0.20	4/90313 (0.0%)	0.38	12/129266 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	2	1650	C	O3'-P	-21.93	1.28	1.61
37	2	921	G	O3'-P	14.79	1.83	1.61
21	U	42	ASN	CA-C	-5.67	1.45	1.52
21	U	40	ARG	CA-C	-5.59	1.45	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	2	1650	C	P-O3'-C3'	12.01	138.22	120.20
28	a	211	LYS	N-CA-C	-8.81	101.61	114.39
2	B	212	PRO	CA-N-CD	-8.71	99.81	112.00
16	P	3	PRO	CA-N-CD	-8.68	99.84	112.00
37	2	1650	C	O3'-P-O5'	8.60	116.90	104.00
28	a	209	TRP	N-CA-C	-8.53	97.26	109.96
28	a	284	PRO	N-CA-CB	7.52	110.37	103.08
21	U	42	ASN	N-CA-C	-6.96	99.20	110.20
3	C	280	PRO	N-CA-CB	6.77	110.45	103.00
28	a	285	PRO	N-CA-CB	6.72	110.43	103.38
28	a	239	PRO	N-CA-CB	6.30	109.75	102.88
33	f	157	ILE	CB-CA-C	-5.10	108.94	114.35

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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	1611	0	1633	13	0
2	B	3877	0	4008	154	0
3	C	2806	0	2971	29	0
4	D	3425	0	3451	25	0
5	E	823	0	879	4	0
6	F	1254	0	1268	16	0
7	G	1037	0	1058	10	0
8	H	1662	0	1700	17	0
9	I	941	0	970	13	0
10	J	993	0	1034	27	0
11	K	992	0	1051	14	0
12	L	864	0	891	5	0
13	M	843	0	884	18	0
14	N	941	0	978	3	0
15	O	869	0	898	6	0
16	P	717	0	755	8	0
17	Q	724	0	744	22	0
18	R	1299	0	1307	8	0
19	S	611	0	687	18	0
20	T	408	0	444	2	0
21	U	1016	0	1062	19	0
22	V	1399	0	1427	15	0
23	W	3062	0	3029	35	0
24	X	1613	0	1559	66	0
25	Y	793	0	834	15	0
26	Z	660	0	675	7	0
27	7	2878	0	2946	41	0
28	a	2486	0	2376	109	0
29	b	581	0	592	21	0
30	c	232	0	278	2	0
31	d	616	0	674	5	0
32	e	2074	0	2074	16	0
33	f	2898	0	2852	80	0
34	h	2463	0	2488	66	0
35	i	2487	0	2450	21	0
36	k	177	0	179	2	0
37	2	33424	0	16844	214	0
38	2	9	0	0	0	0
38	K	1	0	0	0	0
39	2	82	0	0	0	0
39	7	1	0	0	0	0
39	T	1	0	0	0	0
39	W	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	W	31	0	12	0	0
41	7	1	0	0	0	0
42	7	32	0	12	0	0
All	All	85715	0	69974	882	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 6.

All (882) 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)
2:B:231:ARG:HD3	24:X:426:GLU:CD	1.22	1.53
19:S:93:ILE:CG2	29:b:86:LEU:HD13	1.02	1.49
19:S:93:ILE:HG21	29:b:86:LEU:CD1	1.02	1.47
2:B:231:ARG:CD	24:X:426:GLU:OE1	1.66	1.43
34:h:302:HIS:CE1	34:h:356:SER:HB3	1.58	1.38
2:B:249:MET:CE	28:a:358:GLU:OE2	1.74	1.35
2:B:249:MET:HE1	28:a:358:GLU:OE2	1.28	1.33
2:B:231:ARG:CD	24:X:426:GLU:CD	2.04	1.28
2:B:243:PHE:CE2	24:X:393:LEU:HD21	1.79	1.18
33:f:337:ARG:HH22	33:f:389:THR:CG2	1.56	1.17
33:f:389:THR:CG2	33:f:397:GLU:HB3	1.74	1.16
2:B:231:ARG:HD2	24:X:426:GLU:OE1	1.41	1.16
27:7:28:LEU:HB3	27:7:29:PRO:HD2	1.28	1.13
33:f:337:ARG:HH22	33:f:389:THR:HG23	1.12	1.11
19:S:93:ILE:HD13	29:b:86:LEU:HD12	1.34	1.08
13:M:142:MET:HE1	13:M:150:LEU:HD12	1.09	1.08
24:X:492:VAL:HG12	24:X:511:MET:HE1	1.36	1.07
13:M:142:MET:CE	13:M:150:LEU:HD12	1.85	1.05
33:f:337:ARG:NH2	33:f:389:THR:HG23	1.71	1.04
33:f:389:THR:HG21	33:f:397:GLU:HB3	1.39	1.01
3:C:139:VAL:HG11	3:C:144:LEU:HD22	1.43	1.01
34:h:93:ILE:HD11	34:h:108:LEU:HB3	1.41	1.01
34:h:302:HIS:CE1	34:h:356:SER:CB	2.44	1.00
19:S:93:ILE:HD13	29:b:86:LEU:CD1	1.90	0.99
27:7:204:ARG:HH21	27:7:276:ILE:HD13	1.25	0.99
2:B:249:MET:SD	28:a:358:GLU:OE2	2.21	0.98
2:B:376:VAL:HG12	2:B:380:ILE:HG23	1.47	0.97
2:B:110:LEU:HG	28:a:121:VAL:HG22	1.45	0.96
13:M:142:MET:HE1	13:M:150:LEU:CD1	1.94	0.96
2:B:231:ARG:HB3	24:X:426:GLU:OE2	1.63	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:f:253:SER:HB3	35:i:283:TYR:OH	1.66	0.95
28:a:128:GLN:NE2	37:2:1028:A:N7	2.15	0.94
2:B:110:LEU:HG	28:a:121:VAL:CG2	1.97	0.94
25:Y:14:VAL:HG11	28:a:330:ARG:HD2	1.48	0.93
2:B:243:PHE:CE2	24:X:393:LEU:CD2	2.51	0.93
2:B:243:PHE:CZ	24:X:393:LEU:HD21	2.05	0.92
33:f:230:VAL:HG22	33:f:252:TYR:HB3	1.48	0.92
2:B:231:ARG:HD3	24:X:426:GLU:OE2	1.69	0.91
2:B:231:ARG:HD3	24:X:426:GLU:OE1	1.38	0.91
34:h:322:LYS:HZ2	34:h:326:LEU:CD1	1.83	0.91
34:h:302:HIS:HE1	34:h:356:SER:HB3	1.35	0.91
17:Q:193:LEU:HD21	17:Q:213:ILE:HG21	1.53	0.90
27:7:28:LEU:HB3	27:7:29:PRO:CD	2.02	0.90
19:S:97:LYS:HZ1	29:b:86:LEU:HB3	1.35	0.90
10:J:188:ASN:ND2	17:Q:250:ILE:HG22	1.87	0.89
33:f:58:ARG:NE	33:f:61:SER:OG	2.06	0.89
11:K:31:LEU:HD12	11:K:80:VAL:O	1.71	0.89
2:B:481:ARG:NE	28:a:155:ASP:OD2	2.05	0.89
28:a:192:ILE:HG22	28:a:193:LEU:HD22	1.53	0.88
10:J:188:ASN:HB3	17:Q:250:ILE:HG21	1.55	0.87
2:B:363:LEU:HB3	24:X:360:TYR:OH	1.76	0.86
27:7:373:GLY:O	37:2:1472:C:H4'	1.76	0.86
2:B:295:SER:CB	28:a:209:TRP:CH2	2.59	0.85
19:S:97:LYS:NZ	29:b:86:LEU:HB3	1.91	0.85
2:B:110:LEU:HD21	28:a:121:VAL:CG2	2.05	0.85
2:B:110:LEU:CG	28:a:121:VAL:CG2	2.55	0.84
27:7:163:CYS:SG	27:7:171:LEU:HD13	2.17	0.84
2:B:292:PHE:HD1	28:a:209:TRP:HZ3	1.25	0.84
24:X:492:VAL:HG12	24:X:511:MET:CE	2.06	0.83
33:f:128:ASN:OD1	33:f:400:LEU:HD23	1.79	0.83
33:f:337:ARG:CZ	33:f:389:THR:HG23	2.08	0.83
2:B:62:LEU:CD2	2:B:71:ILE:HG12	2.08	0.83
2:B:231:ARG:CB	24:X:426:GLU:OE2	2.25	0.83
2:B:110:LEU:CD2	28:a:121:VAL:CG2	2.57	0.83
33:f:337:ARG:NH2	33:f:389:THR:CG2	2.36	0.83
9:I:232:SER:O	28:a:376:ALA:HB1	1.77	0.82
33:f:337:ARG:HH12	33:f:389:THR:HG23	1.43	0.82
34:h:322:LYS:HZ2	34:h:326:LEU:HD12	1.40	0.82
33:f:337:ARG:NH1	33:f:389:THR:HG23	1.93	0.82
19:S:93:ILE:CB	29:b:86:LEU:HD13	2.09	0.82
19:S:93:ILE:HG21	29:b:86:LEU:CG	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:188:ASN:HB3	17:Q:250:ILE:CG2	2.10	0.81
33:f:389:THR:HG22	33:f:397:GLU:HB3	1.61	0.81
13:M:150:LEU:CD2	13:M:155:GLU:OE1	2.30	0.80
24:X:492:VAL:CG1	24:X:511:MET:HE1	2.13	0.78
34:h:93:ILE:HD11	34:h:108:LEU:CB	2.13	0.78
2:B:480:LYS:O	2:B:481:ARG:CB	2.32	0.78
24:X:409:MET:HB2	24:X:410:PRO:HD2	1.66	0.78
16:P:29:LEU:HD11	37:2:562:C:C4	2.19	0.77
37:2:26:U:H3	37:2:910:G:H1	1.31	0.77
2:B:292:PHE:HA	28:a:209:TRP:CZ3	2.21	0.76
34:h:169:ARG:NH1	34:h:172:TRP:CH2	2.54	0.76
24:X:440:GLU:O	24:X:444:GLU:HG2	1.85	0.76
33:f:323:GLY:HA3	33:f:334:ARG:HH21	1.48	0.76
34:h:322:LYS:NZ	34:h:326:LEU:CD1	2.48	0.76
27:7:204:ARG:NH2	27:7:276:ILE:HD13	2.00	0.76
33:f:337:ARG:HH22	33:f:389:THR:HG21	1.47	0.76
37:2:1650:C:O2'	37:2:1651:C:H5'	1.85	0.75
21:U:95:ASN:OD1	35:i:389:LYS:HG3	1.85	0.75
28:a:213:LEU:O	28:a:218:LYS:NZ	2.20	0.75
2:B:295:SER:HB3	28:a:209:TRP:CZ2	2.20	0.75
29:b:21:ILE:HG23	37:2:1845:A:N6	2.01	0.75
28:a:151:ASP:OD1	28:a:151:ASP:O	2.05	0.74
2:B:295:SER:OG	28:a:209:TRP:CH2	2.39	0.74
34:h:302:HIS:HE1	34:h:356:SER:CB	1.95	0.74
10:J:200:LEU:HD23	10:J:205:THR:HG23	1.68	0.74
2:B:110:LEU:HD21	28:a:121:VAL:HG21	1.68	0.74
2:B:292:PHE:HD1	28:a:209:TRP:CZ3	2.06	0.73
34:h:302:HIS:HA	34:h:360:ASP:OD2	1.89	0.73
28:a:293:TRP:CZ3	28:a:315:LEU:HD13	2.24	0.73
2:B:109:CYS:SG	28:a:124:SER:OG	2.31	0.72
33:f:103:ASP:O	33:f:106:PRO:HD2	1.90	0.72
2:B:110:LEU:CG	28:a:121:VAL:HG21	2.20	0.71
27:7:372:VAL:O	37:2:1471:C:O2'	2.08	0.71
21:U:67:LYS:HB3	21:U:69:VAL:HG23	1.73	0.71
24:X:366:ARG:HH12	28:a:126:GLN:HE21	1.38	0.71
33:f:323:GLY:HA3	33:f:334:ARG:NH2	2.06	0.70
37:2:609:U:H3	37:2:625:G:H22	1.37	0.70
21:U:113:GLU:HG3	21:U:117:LYS:HE2	1.73	0.70
2:B:230:VAL:HG21	24:X:444:GLU:HG3	1.72	0.70
33:f:105:LEU:N	33:f:106:PRO:HD2	2.06	0.70
2:B:231:ARG:CD	24:X:426:GLU:OE2	2.32	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:295:SER:HB3	28:a:209:TRP:CH2	2.27	0.70
25:Y:14:VAL:CG1	28:a:330:ARG:HD2	2.21	0.69
2:B:110:LEU:HD21	28:a:121:VAL:HG23	1.73	0.69
2:B:490:SER:O	2:B:533:LEU:HD12	1.93	0.69
3:C:139:VAL:HG11	3:C:144:LEU:CD2	2.22	0.69
37:2:858:A:H5'	37:2:1070:U:O4	1.91	0.69
2:B:480:LYS:O	2:B:481:ARG:HB3	1.92	0.68
37:2:1524:A:H2	37:2:1537:G:H21	1.40	0.68
2:B:295:SER:CB	28:a:209:TRP:HH2	2.06	0.68
24:X:477:VAL:HG13	24:X:478:PRO:HD2	1.74	0.68
34:h:323:LYS:O	34:h:327:GLU:HG3	1.93	0.68
34:h:203:ASP:OD1	34:h:236:LEU:HD12	1.93	0.68
13:M:150:LEU:HD23	13:M:155:GLU:OE1	1.94	0.67
19:S:93:ILE:CD1	29:b:86:LEU:CD1	2.71	0.67
33:f:58:ARG:NE	33:f:61:SER:CB	2.58	0.67
21:U:89:VAL:O	21:U:93:THR:HG23	1.95	0.67
2:B:364:ARG:HG2	24:X:360:TYR:CE2	2.30	0.67
27:7:24:ASN:OD1	27:7:25:PRO:HD2	1.95	0.67
18:R:140:PRO:HB2	18:R:164:THR:HG21	1.77	0.67
33:f:153:GLY:O	33:f:157:ILE:HG12	1.94	0.67
34:h:194:LEU:HA	34:h:227:ILE:HD13	1.77	0.67
17:Q:186:PHE:O	17:Q:194:VAL:HG22	1.95	0.67
17:Q:166:ILE:HD11	17:Q:185:GLN:OE1	1.95	0.66
2:B:191:ILE:CD1	28:a:192:ILE:CD1	2.73	0.66
2:B:288:ARG:HD3	28:a:212:LEU:CB	2.24	0.66
25:Y:43:ARG:NH1	37:2:1537:G:N7	2.42	0.66
37:2:660:G:H22	37:2:737:G:H1	1.41	0.66
2:B:110:LEU:HD11	28:a:121:VAL:HG21	1.78	0.66
9:I:224:LEU:HB2	28:a:291:LEU:HD21	1.78	0.66
1:A:151:LYS:HD3	37:2:1067:U:OP1	1.96	0.66
11:K:114:ARG:HB2	11:K:119:ALA:HB3	1.79	0.65
37:2:83:U:H3	37:2:157:G:H1	1.43	0.65
10:J:188:ASN:ND2	17:Q:250:ILE:CG2	2.60	0.65
34:h:159:VAL:HG13	34:h:192:TYR:HB2	1.77	0.64
27:7:369:ARG:NH1	37:2:1046:C:O2'	2.29	0.64
2:B:110:LEU:CD2	28:a:121:VAL:HG23	2.26	0.64
2:B:288:ARG:HD3	28:a:212:LEU:HB3	1.79	0.64
2:B:62:LEU:HD22	2:B:71:ILE:HG12	1.79	0.64
2:B:460:LEU:HD13	2:B:533:LEU:CD2	2.28	0.64
34:h:260:MET:SD	34:h:279:ARG:NH2	2.71	0.64
16:P:3:PRO:HD2	16:P:3:PRO:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:7:220:SER:O	27:7:224:ILE:HG12	1.97	0.64
34:h:322:LYS:NZ	34:h:326:LEU:HD11	2.11	0.64
2:B:292:PHE:CD1	28:a:209:TRP:HZ3	2.14	0.63
16:P:2:LYS:HB3	16:P:3:PRO:CD	2.29	0.63
37:2:200:C:H5	37:2:246:G:H1	1.47	0.63
2:B:151:LYS:HG2	24:X:458:PRO:HD2	1.80	0.63
2:B:371:LEU:HD21	28:a:102:ILE:HG21	1.80	0.63
13:M:150:LEU:HD22	13:M:155:GLU:OE1	1.99	0.63
37:2:1719:G:H1	37:2:1752:U:H3	1.45	0.63
33:f:268:GLU:O	33:f:272:ARG:HG3	1.98	0.62
37:2:969:G:H22	37:2:1625:A:H5'	1.63	0.62
2:B:343:LEU:HD22	24:X:376:LEU:CD2	2.29	0.62
37:2:1669:C:H2'	37:2:1670:A:H8	1.63	0.62
2:B:110:LEU:O	2:B:111:ARG:HB2	2.00	0.62
2:B:395:VAL:HG13	28:a:105:LEU:HD23	1.81	0.62
33:f:249:LEU:O	33:f:253:SER:OG	2.13	0.62
34:h:266:ARG:HG3	34:h:268:ASP:H	1.65	0.62
2:B:170:SER:OG	2:B:174:ARG:NH1	2.33	0.62
29:b:21:ILE:HG23	37:2:1845:A:H61	1.65	0.61
24:X:410:PRO:HG2	24:X:413:GLU:HG3	1.82	0.61
25:Y:6:LEU:O	25:Y:10:VAL:HG23	2.00	0.61
1:A:70:VAL:HG21	1:A:145:VAL:HG21	1.83	0.61
2:B:191:ILE:CD1	28:a:192:ILE:HD13	2.30	0.61
8:H:415:LYS:HE3	37:2:1450:G:H5'	1.82	0.61
33:f:128:ASN:OD1	33:f:400:LEU:CD2	2.48	0.61
33:f:39:VAL:HG12	33:f:72:ARG:HD3	1.82	0.61
30:c:112:ASP:N	37:2:571:A:OP1	2.34	0.61
37:2:670:G:H2'	37:2:671:A:H8	1.65	0.61
34:h:259:TRP:HE1	34:h:275:VAL:HG11	1.66	0.61
37:2:968:A:H4'	37:2:969:G:H5''	1.83	0.61
1:A:16:SER:HB2	1:A:178:ALA:HB1	1.82	0.61
25:Y:15:THR:HB	28:a:334:GLU:HG2	1.81	0.61
34:h:288:LEU:HD11	34:h:326:LEU:HD21	1.81	0.61
25:Y:14:VAL:HG13	25:Y:15:THR:HG23	1.83	0.60
2:B:526:VAL:HB	2:B:533:LEU:HB3	1.83	0.60
17:Q:227:MET:HE3	19:S:52:MET:HG2	1.83	0.60
33:f:103:ASP:C	33:f:106:PRO:HD2	2.26	0.60
24:X:488:PHE:O	24:X:492:VAL:HG23	2.01	0.60
27:7:375:MET:N	37:2:1473:C:OP1	2.32	0.60
2:B:13:GLY:HA2	13:M:160:LYS:NZ	2.16	0.60
2:B:343:LEU:HD22	24:X:376:LEU:HD23	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:f:103:ASP:O	33:f:106:PRO:CG	2.49	0.60
10:J:279:ARG:NH1	10:J:283:SER:OG	2.34	0.60
2:B:249:MET:HE1	28:a:358:GLU:CD	2.20	0.60
17:Q:166:ILE:CD1	17:Q:185:GLN:OE1	2.50	0.60
2:B:295:SER:OG	28:a:209:TRP:HH2	1.83	0.60
4:D:370:VAL:HG11	37:2:1072:A:H5''	1.83	0.60
33:f:147:VAL:HG21	35:i:315:THR:HG21	1.83	0.60
2:B:284:ARG:HE	2:B:288:ARG:HH21	1.48	0.59
3:C:133:CYS:SG	3:C:155:GLN:NE2	2.74	0.59
28:a:293:TRP:CE3	28:a:315:LEU:HD13	2.37	0.59
24:X:366:ARG:NH1	28:a:126:GLN:HE21	2.00	0.59
2:B:212:PRO:HD2	2:B:212:PRO:O	2.02	0.59
33:f:103:ASP:O	33:f:106:PRO:CD	2.51	0.59
2:B:110:LEU:CD2	28:a:121:VAL:HG21	2.27	0.59
3:C:204:THR:HA	4:D:116:GLU:HG2	1.85	0.59
2:B:461:LYS:NZ	2:B:527:SER:OG	2.36	0.59
33:f:105:LEU:N	33:f:106:PRO:CD	2.66	0.59
33:f:389:THR:HG21	33:f:397:GLU:CB	2.23	0.59
29:b:22:ASN:HB3	29:b:25:LYS:HB2	1.83	0.59
37:2:1734:A:H2'	37:2:1735:C:H4'	1.84	0.59
2:B:14:LYS:NZ	37:2:1106:C:OP1	2.35	0.59
19:S:93:ILE:CD1	29:b:86:LEU:HD12	2.23	0.59
24:X:366:ARG:NH1	28:a:126:GLN:NE2	2.50	0.59
34:h:171:LEU:O	34:h:212:ASN:ND2	2.35	0.59
34:h:338:PRO:HA	34:h:341:VAL:HG12	1.85	0.59
2:B:376:VAL:HG12	2:B:376:VAL:O	2.03	0.59
2:B:383:PHE:HD1	2:B:389:ILE:HD11	1.68	0.59
13:M:142:MET:CE	13:M:150:LEU:CD1	2.70	0.58
27:7:393:SER:O	27:7:397:VAL:HG23	2.03	0.58
2:B:299:GLU:H	2:B:309:ARG:HH22	1.51	0.58
2:B:371:LEU:CD2	28:a:102:ILE:HG21	2.33	0.58
22:V:39:GLU:HG3	22:V:40:THR:HG23	1.85	0.58
28:a:213:LEU:HD22	28:a:217:LEU:HD22	1.86	0.58
33:f:120:LYS:HE2	33:f:340:LEU:HD11	1.85	0.58
2:B:525:GLU:OE1	37:2:1049:G:O2'	2.20	0.58
33:f:310:PRO:HB3	33:f:373:LEU:HD13	1.85	0.58
34:h:241:SER:O	34:h:245:CYS:SG	2.62	0.58
33:f:337:ARG:HH12	33:f:389:THR:CG2	2.15	0.57
23:W:372:THR:HB	23:W:375:SER:HB3	1.86	0.57
2:B:110:LEU:CD1	28:a:121:VAL:HG21	2.34	0.57
2:B:383:PHE:CD1	2:B:389:ILE:HD11	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:251:LYS:HD3	10:J:282:TYR:CE1	2.39	0.57
37:2:836:A:O2'	37:2:839:C:N4	2.31	0.57
37:2:939:A:H2'	37:2:940:G:C8	2.39	0.57
3:C:17:LEU:HD13	37:2:451:A:H4'	1.84	0.57
34:h:263:ALA:HA	34:h:266:ARG:HE	1.69	0.57
27:7:347:ASP:O	27:7:351:VAL:HG23	2.05	0.57
12:L:33:ARG:NH1	12:L:38:GLU:OE2	2.37	0.57
28:a:179:LYS:O	28:a:183:ILE:HG13	2.04	0.57
37:2:1839:G:H2'	37:2:1840:A:H8	1.69	0.57
34:h:93:ILE:HG23	34:h:104:PRO:HG3	1.87	0.57
18:R:175:ARG:HB3	18:R:182:HIS:HB3	1.86	0.57
27:7:91:VAL:HG12	27:7:108:VAL:HG12	1.87	0.57
33:f:157:ILE:HG21	33:f:188:TYR:CG	2.40	0.57
34:h:152:ARG:NH1	37:2:1729:G:H1'	2.20	0.56
3:C:162:ARG:NH2	3:C:165:GLU:OE1	2.38	0.56
4:D:187:LEU:HB3	35:i:237:ARG:HG2	1.87	0.56
15:O:79:ARG:HG2	32:e:334:ILE:HD12	1.86	0.56
10:J:188:ASN:CB	17:Q:250:ILE:HG21	2.32	0.56
23:W:208:GLN:NE2	23:W:397:ASP:O	2.38	0.56
24:X:421:PHE:HB2	28:a:206:MET:HE1	1.86	0.56
28:a:293:TRP:CH2	28:a:315:LEU:HD13	2.41	0.56
33:f:253:SER:HB3	35:i:283:TYR:CZ	2.40	0.56
33:f:356:ARG:NH1	33:f:361:ASP:OD2	2.38	0.56
2:B:111:ARG:O	2:B:111:ARG:HG2	2.05	0.56
27:7:190:VAL:HG13	27:7:224:ILE:HG13	1.87	0.56
2:B:108:GLY:O	2:B:109:CYS:C	2.49	0.56
2:B:191:ILE:CD1	28:a:192:ILE:HD11	2.34	0.56
3:C:107:PHE:HD1	3:C:146:LEU:HD11	1.71	0.56
6:F:31:ILE:HD13	6:F:107:LEU:HD23	1.87	0.56
29:b:21:ILE:HG23	37:2:1845:A:C6	2.41	0.56
34:h:288:LEU:HD11	34:h:326:LEU:HD11	1.88	0.56
36:k:12:ASN:HB3	36:k:15:LYS:HE3	1.87	0.56
37:2:58:A:O2'	37:2:379:G:N2	2.38	0.56
22:V:184:LYS:HA	22:V:187:GLU:HG2	1.88	0.55
37:2:920:G:OP1	37:2:1814:G:N2	2.37	0.55
1:A:151:LYS:CD	37:2:1067:U:OP1	2.54	0.55
34:h:105:PRO:HG3	37:2:1717:C:H4'	1.88	0.55
9:I:206:ARG:HG3	24:X:386:ILE:HG21	1.87	0.55
8:H:224:VAL:HG12	8:H:225:ILE:H	1.72	0.55
8:H:395:ARG:NH2	37:2:1442:A:OP2	2.39	0.55
33:f:58:ARG:CD	33:f:61:SER:HB2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:f:232:GLU:OE2	33:f:236:LYS:NZ	2.39	0.55
37:2:1430:A:O2'	37:2:1432:A:N7	2.40	0.55
4:D:145:SER:HB2	4:D:148:SER:HB2	1.88	0.55
22:V:113:ARG:NH1	37:2:635:G:O2'	2.40	0.55
28:a:333:ARG:NH2	37:2:1131:G:OP1	2.40	0.55
33:f:230:VAL:HG22	33:f:252:TYR:CB	2.32	0.55
33:f:253:SER:CB	35:i:283:TYR:CZ	2.90	0.55
2:B:309:ARG:HA	2:B:312:HIS:HB3	1.88	0.55
3:C:182:LYS:HB3	3:C:309:ILE:HD12	1.88	0.55
7:G:22:ALA:HB2	21:U:41:SER:HA	1.89	0.55
28:a:128:GLN:NE2	37:2:1028:A:C5	2.75	0.54
6:F:105:ILE:HB	6:F:109:LYS:HD3	1.90	0.54
37:2:151:A:H5''	37:2:152:G:H5'	1.88	0.54
4:D:381:ARG:HE	4:D:401:LYS:HD3	1.73	0.54
37:2:883:G:O2'	37:2:899:A:N6	2.39	0.54
2:B:460:LEU:HD13	2:B:533:LEU:HD23	1.89	0.54
10:J:188:ASN:CB	17:Q:250:ILE:CG2	2.83	0.54
37:2:1705:C:N4	37:2:1763:U:OP2	2.38	0.54
23:W:271:LEU:HD22	23:W:322:VAL:HG13	1.88	0.54
24:X:401:PRO:HG3	28:a:361:ARG:HD2	1.89	0.54
34:h:184:ALA:O	34:h:188:HIS:ND1	2.40	0.54
8:H:311:ARG:H	8:H:381:LEU:HD23	1.72	0.54
10:J:246:ILE:O	10:J:250:VAL:HG23	2.08	0.54
27:7:386:PRO:HA	27:7:390:ARG:HB2	1.90	0.54
37:2:1567:G:H21	37:2:1594:A:H2	1.55	0.54
33:f:58:ARG:CZ	33:f:61:SER:OG	2.56	0.53
33:f:241:ASP:OD2	33:f:243:THR:OG1	2.25	0.53
33:f:323:GLY:CA	33:f:334:ARG:NH2	2.72	0.53
2:B:243:PHE:HE2	24:X:393:LEU:CD2	2.17	0.53
23:W:215:VAL:HG22	23:W:216:LYS:HG2	1.89	0.53
27:7:39:ALA:HA	27:7:44:MET:HG2	1.91	0.53
33:f:83:ASN:O	33:f:138:LYS:NZ	2.41	0.53
33:f:279:VAL:HG22	33:f:317:LEU:HD12	1.89	0.53
35:i:191:GLN:HA	35:i:196:MET:HE3	1.91	0.53
2:B:406:LYS:HG3	28:a:90:PHE:HA	1.90	0.53
23:W:223:LEU:HD11	23:W:354:ALA:HB1	1.90	0.53
33:f:63:ASN:ND2	33:f:97:THR:O	2.41	0.53
34:h:234:TRP:HB2	34:h:266:ARG:HH12	1.74	0.53
37:2:1121:U:H5''	37:2:1122:C:H5'	1.90	0.53
3:C:217:LEU:HD23	3:C:220:LEU:HD12	1.91	0.53
27:7:209:VAL:HA	27:7:283:ALA:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:7:86:LEU:HD22	27:7:119:PRO:HB2	1.91	0.52
27:7:386:PRO:HG2	37:2:1459:A:C8	2.44	0.52
33:f:319:SER:OG	33:f:334:ARG:NH1	2.39	0.52
34:h:342:LEU:C	34:h:342:LEU:HD12	2.35	0.52
20:T:96:LYS:HB2	37:2:1400:G:H4'	1.89	0.52
21:U:85:TYR:OH	21:U:103:MET:SD	2.67	0.52
34:h:89:LEU:HD11	34:h:108:LEU:HD22	1.92	0.52
2:B:107:ILE:HD11	28:a:125:LEU:HD21	1.92	0.52
3:C:42:LEU:HD23	3:C:45:LEU:HD12	1.92	0.52
24:X:410:PRO:HD2	24:X:413:GLU:OE1	2.10	0.52
35:i:321:VAL:HA	35:i:324:LYS:HG2	1.91	0.52
21:U:5:LYS:O	21:U:14:ARG:NH2	2.42	0.52
6:F:25:ARG:NH1	37:2:1636:A:OP1	2.42	0.52
15:O:6:ARG:HB2	37:2:395:G:H5''	1.91	0.52
23:W:313:PRO:HD2	23:W:316:SER:HB3	1.90	0.52
33:f:319:SER:CA	33:f:334:ARG:HH12	2.22	0.52
6:F:5:ASP:OD1	6:F:8:GLN:NE2	2.40	0.52
2:B:193:PHE:O	2:B:197:ASN:CB	2.58	0.52
2:B:284:ARG:HH11	28:a:201:GLU:HG3	1.74	0.52
20:T:82:LYS:HE3	23:W:363:THR:HG22	1.92	0.52
10:J:188:ASN:HD22	17:Q:250:ILE:HG22	1.69	0.52
27:7:13:SER:HB2	27:7:379:GLN:HB3	1.91	0.52
35:i:105:VAL:HG13	35:i:128:LEU:HD11	1.92	0.52
2:B:288:ARG:HD3	28:a:212:LEU:HB2	1.90	0.52
13:M:122:ARG:NE	37:2:972:C:O2	2.42	0.52
37:2:385:C:O2'	37:2:386:U:O2	2.26	0.52
27:7:263:ARG:NH2	37:2:787:G:O3'	2.43	0.52
28:a:221:VAL:HG23	28:a:224:LYS:HE2	1.91	0.52
31:d:74:ARG:HD3	37:2:470:C:H5'	1.92	0.52
37:2:1618:G:H2'	37:2:1619:A:C8	2.44	0.52
37:2:669:G:H2'	37:2:670:G:C8	2.45	0.51
37:2:709:G:H2'	37:2:710:G:C8	2.45	0.51
37:2:1703:G:H3'	37:2:1704:A:H8	1.74	0.51
4:D:77:ASP:HA	4:D:80:VAL:HG12	1.92	0.51
23:W:291:ASP:O	23:W:338:ARG:NH1	2.43	0.51
2:B:309:ARG:O	2:B:312:HIS:ND1	2.36	0.51
19:S:93:ILE:CB	29:b:86:LEU:CD1	2.81	0.51
27:7:372:VAL:HG12	37:2:1472:C:H4'	1.93	0.51
27:7:226:ARG:HH22	27:7:249:PHE:HA	1.75	0.51
2:B:108:GLY:O	2:B:110:LEU:N	2.43	0.51
32:e:168:LEU:HA	32:e:171:VAL:HG12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:22:TRP:HB3	2:B:64:HIS:HB2	1.92	0.51
2:B:331:SER:H	28:a:193:LEU:HD11	1.75	0.51
2:B:191:ILE:HD13	28:a:192:ILE:HD13	1.91	0.51
3:C:21:THR:HG21	3:C:77:LEU:HD11	1.91	0.51
33:f:226:ARG:NH1	33:f:254:ASP:OD1	2.43	0.51
33:f:323:GLY:CA	33:f:334:ARG:HH21	2.20	0.51
2:B:359:LEU:O	2:B:363:LEU:HB2	2.11	0.50
2:B:249:MET:SD	28:a:358:GLU:CD	2.94	0.50
33:f:58:ARG:NE	33:f:61:SER:HB2	2.25	0.50
34:h:169:ARG:NH1	34:h:172:TRP:HH2	2.08	0.50
34:h:293:SER:HA	34:h:296:LYS:HD2	1.93	0.50
37:2:328:A:H2'	37:2:329:G:H8	1.76	0.50
16:P:10:SER:HB2	16:P:18:VAL:HB	1.92	0.50
23:W:101:ARG:NH2	23:W:445:GLN:O	2.43	0.50
4:D:217:LEU:HD11	35:i:207:ILE:HD11	1.93	0.50
9:I:205:LYS:HD2	24:X:392:TYR:HB3	1.92	0.50
11:K:35:LEU:HD11	11:K:56:ARG:HG3	1.92	0.50
37:2:164:A:H2'	37:2:165:A:C8	2.47	0.50
37:2:969:G:OP2	37:2:1620:U:O2'	2.30	0.50
9:I:156:MET:HB2	9:I:185:LYS:HB3	1.93	0.50
10:J:203:ASN:HA	10:J:234:MET:HG3	1.93	0.50
34:h:368:LEU:HD22	34:h:373:LEU:HD22	1.94	0.50
1:A:93:ASN:HB3	1:A:96:ARG:HB3	1.92	0.50
6:F:67:GLY:HA2	6:F:72:ILE:HA	1.93	0.50
19:S:80:LYS:HG3	37:2:1846:U:C4	2.46	0.50
37:2:328:A:O2'	37:2:605:A:N1	2.43	0.50
2:B:206:LEU:HD11	28:a:187:GLY:HA2	1.93	0.50
11:K:56:ARG:HH21	11:K:60:ARG:HG3	1.76	0.50
24:X:410:PRO:HG2	24:X:413:GLU:CG	2.42	0.50
5:E:37:LEU:HB2	22:V:176:ILE:HB	1.94	0.50
28:a:180:TRP:HA	28:a:183:ILE:HD12	1.93	0.50
2:B:193:PHE:O	2:B:197:ASN:HB2	2.12	0.50
6:F:100:ARG:NH2	37:2:1502:A:O2'	2.45	0.50
11:K:6:GLN:HG2	11:K:9:ARG:HH21	1.77	0.50
28:a:209:TRP:O	28:a:210:ASP:CB	2.59	0.50
3:C:100:LEU:HD12	3:C:352:LEU:HD21	1.92	0.49
11:K:50:ARG:NH2	11:K:89:ASP:OD2	2.45	0.49
13:M:126:ARG:NH1	13:M:131:GLY:O	2.45	0.49
33:f:266:LYS:HB3	33:f:269:MET:HE3	1.93	0.49
34:h:252:ARG:NH2	37:2:1731:A:OP2	2.34	0.49
37:2:1671:C:H2'	37:2:1672:A:H8	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:31:ILE:HG23	6:F:108:GLU:HG3	1.94	0.49
27:7:27:LEU:HD11	27:7:33:ILE:HG12	1.92	0.49
28:a:294:GLN:HB2	28:a:314:LYS:HB2	1.93	0.49
33:f:286:MET:O	33:f:290:VAL:HG23	2.12	0.49
33:f:319:SER:O	33:f:334:ARG:NH2	2.44	0.49
37:2:673:U:H3	37:2:709:G:H22	1.60	0.49
3:C:287:LEU:HD11	4:D:178:LEU:HB3	1.95	0.49
11:K:114:ARG:NH2	37:2:499:C:OP1	2.45	0.49
33:f:57:ASP:OD1	33:f:94:SER:OG	2.30	0.49
37:2:161:A:H2'	37:2:162:C:H4'	1.94	0.49
9:I:131:CYS:HB2	9:I:217:GLN:HB2	1.93	0.49
12:L:32:ILE:N	12:L:39:VAL:O	2.45	0.49
2:B:480:LYS:O	2:B:481:ARG:HB2	2.13	0.49
28:a:219:LYS:HA	28:a:222:GLU:HG2	1.95	0.49
37:2:993:G:H2'	37:2:994:A:H8	1.78	0.49
23:W:358:TYR:OH	23:W:391:ARG:O	2.30	0.49
24:X:428:ILE:HG23	24:X:433:GLU:HB3	1.95	0.49
37:2:356:G:H2'	37:2:357:A:C8	2.48	0.49
37:2:1689:C:H2'	37:2:1690:G:H8	1.78	0.49
2:B:405:ARG:HG2	28:a:125:LEU:HD22	1.94	0.49
37:2:65:G:H1	37:2:374:C:H5	1.59	0.49
22:V:89:GLU:OE2	22:V:92:ARG:NH2	2.44	0.49
34:h:232:ASP:HA	34:h:262:PHE:HZ	1.77	0.49
37:2:1833:U:H2'	37:2:1834:G:C8	2.48	0.49
37:2:1839:G:H2'	37:2:1840:A:C8	2.48	0.49
9:I:196:GLU:OE2	28:a:177:GLU:OE1	2.31	0.49
17:Q:207:ARG:NH1	37:2:660:G:OP1	2.46	0.49
21:U:34:PRO:HB2	33:f:233:ARG:HH12	1.78	0.49
24:X:430:ASP:N	24:X:430:ASP:OD1	2.44	0.49
30:c:119:LYS:NZ	37:2:881:G:OP2	2.45	0.49
33:f:389:THR:CG2	33:f:397:GLU:CB	2.69	0.49
2:B:62:LEU:HD23	2:B:71:ILE:HG12	1.90	0.48
2:B:288:ARG:CD	28:a:212:LEU:HB3	2.42	0.48
7:G:56:ARG:NH2	22:V:142:GLU:OE1	2.44	0.48
11:K:83:ARG:HB3	11:K:98:ILE:HD11	1.95	0.48
1:A:71:ASN:HB2	1:A:80:VAL:HG11	1.95	0.48
8:H:395:ARG:NH1	37:2:1441:G:OP2	2.46	0.48
2:B:369:ASN:HD21	24:X:335:VAL:HG12	1.77	0.48
5:E:93:LEU:O	37:2:732:U:O2'	2.29	0.48
23:W:210:ILE:HB	23:W:424:ARG:HA	1.94	0.48
33:f:301:THR:O	33:f:305:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:ALA:HB2	1:A:195:CYS:HB3	1.94	0.48
21:U:42:ASN:HD22	21:U:43:GLY:N	2.11	0.48
26:Z:88:LYS:NZ	37:2:215:A:OP1	2.42	0.48
37:2:887:G:H2'	37:2:888:G:C8	2.47	0.48
18:R:35:ILE:HD13	18:R:104:VAL:HG22	1.95	0.48
24:X:381:ASP:OD1	24:X:455:TYR:OH	2.29	0.48
24:X:477:VAL:CG1	24:X:478:PRO:HD2	2.42	0.48
25:Y:84:ARG:HH12	37:2:1470:G:H5''	1.78	0.48
37:2:313:U:OP1	37:2:608:G:O2'	2.27	0.48
37:2:710:G:H2'	37:2:711:A:C8	2.48	0.48
3:C:242:LEU:HD22	3:C:297:PHE:HB3	1.96	0.48
3:C:262:LEU:HD22	32:e:139:MET:HE3	1.96	0.48
17:Q:193:LEU:CD2	17:Q:213:ILE:HG21	2.34	0.48
19:S:93:ILE:HD13	29:b:86:LEU:HD11	1.89	0.48
22:V:121:ALA:O	22:V:124:ARG:NH1	2.47	0.48
25:Y:25:ILE:HG21	28:a:371:LEU:HD12	1.96	0.48
2:B:357:GLU:O	2:B:361:ASN:ND2	2.46	0.48
17:Q:193:LEU:HD21	17:Q:213:ILE:CG2	2.34	0.48
23:W:382:ARG:NH1	23:W:383:GLU:OE2	2.46	0.48
24:X:409:MET:HB2	24:X:410:PRO:CD	2.42	0.48
27:7:137:LEU:HD11	27:7:142:LEU:HD22	1.96	0.48
35:i:134:LYS:HE3	35:i:155:SER:HB2	1.96	0.48
8:H:219:LYS:HZ3	21:U:123:ARG:HB3	1.78	0.48
24:X:403:ILE:HD11	28:a:365:LEU:HD23	1.96	0.48
34:h:165:ASN:O	34:h:169:ARG:HG3	2.13	0.48
37:2:785:U:N3	37:2:788:A:OP2	2.36	0.48
3:C:28:ASN:ND2	4:D:146:SER:O	2.46	0.48
7:G:52:HIS:HB2	7:G:59:ARG:HG3	1.96	0.48
2:B:249:MET:SD	28:a:358:GLU:CG	3.02	0.48
2:B:376:VAL:CG1	2:B:380:ILE:HG23	2.33	0.48
3:C:143:HIS:O	3:C:145:LYS:NZ	2.40	0.48
11:K:35:LEU:HD12	11:K:54:LYS:HG2	1.95	0.48
11:K:110:ARG:NH2	37:2:535:G:OP1	2.46	0.48
8:H:387:LEU:HD22	8:H:394:MET:HE1	1.95	0.47
22:V:36:HIS:O	22:V:40:THR:OG1	2.28	0.47
33:f:103:ASP:O	33:f:106:PRO:HG2	2.12	0.47
34:h:279:ARG:NH1	34:h:294:CYS:SG	2.87	0.47
35:i:105:VAL:HA	35:i:108:MET:HG2	1.95	0.47
37:2:1033:C:H2'	37:2:1034:A:H8	1.78	0.47
2:B:247:ASN:OD1	24:X:460:ARG:NH2	2.47	0.47
37:2:64:U:H2'	37:2:65:G:C8	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:2:613:C:H2'	37:2:614:A:C8	2.49	0.47
37:2:1412:C:H2'	37:2:1413:A:H8	1.80	0.47
4:D:357:ARG:NH1	21:U:20:ALA:O	2.41	0.47
10:J:191:THR:OG1	17:Q:242:ASP:O	2.31	0.47
10:J:188:ASN:CG	17:Q:250:ILE:CG2	2.87	0.47
1:A:10:LYS:HD2	8:H:246:LEU:HG	1.96	0.47
37:2:1702:G:H2'	37:2:1703:G:C8	2.49	0.47
11:K:8:ILE:HG12	16:P:27:ASN:HD22	1.79	0.47
17:Q:227:MET:HG3	19:S:52:MET:HE2	1.97	0.47
26:Z:53:LEU:HB3	26:Z:116:VAL:HG13	1.95	0.47
33:f:253:SER:CB	35:i:283:TYR:OH	2.51	0.47
4:D:236:ILE:HB	32:e:171:VAL:HG21	1.97	0.47
10:J:298:THR:HG22	17:Q:228:GLY:HA2	1.97	0.47
12:L:135:ALA:HB3	12:L:139:LYS:HE3	1.95	0.47
21:U:61:ARG:O	21:U:61:ARG:HG2	2.13	0.47
27:7:189:SER:O	27:7:193:LYS:N	2.47	0.47
28:a:387:THR:HA	28:a:390:VAL:HG12	1.97	0.47
34:h:203:ASP:OD1	34:h:236:LEU:CD1	2.62	0.47
37:2:1650:C:H2'	37:2:1651:C:C6	2.49	0.47
9:I:170:HIS:CE1	9:I:171:VAL:HG22	2.50	0.47
15:O:21:MET:HE1	15:O:36:VAL:HG22	1.96	0.47
15:O:29:ARG:NH1	37:2:409:U:O2'	2.47	0.47
37:2:254:U:H2'	37:2:255:G:H8	1.80	0.47
37:2:1013:A:H2	37:2:1482:U:H1'	1.80	0.47
2:B:292:PHE:CD1	28:a:209:TRP:CZ3	2.95	0.47
6:F:16:VAL:HG22	6:F:32:VAL:HG11	1.97	0.47
2:B:61:ILE:HB	2:B:72:HIS:HB2	1.97	0.46
28:a:192:ILE:HG22	28:a:193:LEU:CD2	2.37	0.46
33:f:58:ARG:NH1	33:f:103:ASP:OD2	2.48	0.46
37:2:902:A:N3	37:2:1675:C:O2'	2.47	0.46
22:V:114:ARG:NH2	37:2:635:G:OP1	2.47	0.46
37:2:939:A:H2'	37:2:940:G:H8	1.79	0.46
2:B:332:LEU:HG	28:a:184:VAL:HG11	1.97	0.46
3:C:25:LEU:HA	3:C:70:GLN:HE22	1.81	0.46
23:W:187:PHE:HA	23:W:190:ILE:HG22	1.97	0.46
28:a:352:GLU:OE2	37:2:1541:G:N2	2.37	0.46
33:f:319:SER:CB	33:f:334:ARG:HH12	2.28	0.46
34:h:152:ARG:HH11	37:2:1729:G:H1'	1.78	0.46
34:h:217:GLN:NE2	37:2:1730:U:O2'	2.45	0.46
37:2:1549:A:H2'	37:2:1550:A:C8	2.50	0.46
37:2:1667:G:O2'	37:2:1827:MA6:O2'	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:110:LEU:O	2:B:111:ARG:CB	2.64	0.46
23:W:174:LEU:HG	23:W:221:ILE:HD11	1.96	0.46
23:W:214:PRO:HG2	23:W:429:ARG:HG3	1.98	0.46
34:h:125:LEU:HD21	34:h:154:VAL:HG23	1.98	0.46
24:X:401:PRO:HD2	28:a:365:LEU:HD22	1.96	0.46
27:7:193:LYS:NZ	27:7:224:ILE:HD12	2.31	0.46
27:7:373:GLY:O	37:2:1472:C:C4'	2.57	0.46
31:d:60:LEU:HD21	31:d:83:ILE:HD11	1.97	0.46
33:f:329:ASP:OD1	33:f:329:ASP:N	2.47	0.46
37:2:1701:C:H2'	37:2:1702:G:H8	1.81	0.46
2:B:44:SER:O	25:Y:69:ARG:NH1	2.46	0.46
33:f:221:PHE:CE2	33:f:256:VAL:HG11	2.51	0.46
34:h:322:LYS:HZ3	34:h:326:LEU:HD11	1.81	0.46
16:P:2:LYS:HB3	16:P:3:PRO:HD3	1.97	0.46
25:Y:10:VAL:HA	28:a:385:ILE:HD11	1.98	0.46
28:a:208:HIS:O	28:a:209:TRP:C	2.56	0.46
2:B:253:PRO:HG3	24:X:414:CYS:HB2	1.96	0.46
2:B:254:VAL:HG11	28:a:207:LEU:HD23	1.98	0.46
7:G:88:TYR:O	7:G:92:THR:OG1	2.29	0.46
23:W:289:VAL:HG13	23:W:338:ARG:HE	1.81	0.46
23:W:451:GLU:HG2	23:W:452:VAL:HG13	1.98	0.46
31:d:46:LEU:HD11	31:d:60:LEU:HD12	1.98	0.46
37:2:241:U:H2'	37:2:242:G:H8	1.81	0.46
3:C:108:ASP:OD1	3:C:108:ASP:N	2.48	0.46
16:P:3:PRO:O	16:P:3:PRO:CD	2.62	0.46
18:R:67:VAL:N	37:2:1136:A:OP1	2.45	0.46
22:V:119:GLU:HA	22:V:122:LYS:HD2	1.98	0.46
25:Y:94:GLY:O	25:Y:96:ARG:N	2.49	0.46
26:Z:57:ALA:HA	26:Z:60:LEU:HD23	1.98	0.46
33:f:234:ILE:HD12	33:f:237:LEU:HD12	1.97	0.46
34:h:269:THR:HA	34:h:272:LEU:HD12	1.97	0.46
37:2:1113:U:H2'	37:2:1114:G:C8	2.50	0.46
7:G:105:THR:OG1	7:G:108:GLY:O	2.29	0.46
8:H:406:ARG:NH1	8:H:407:ASP:O	2.49	0.46
26:Z:52:ASN:ND2	26:Z:55:GLU:OE2	2.49	0.46
27:7:24:ASN:OD1	27:7:25:PRO:CD	2.64	0.46
32:e:239:ASP:OD1	32:e:243:ARG:NH1	2.49	0.46
37:2:1653:U:H2'	37:2:1654:G:C8	2.51	0.46
2:B:231:ARG:NE	24:X:426:GLU:OE1	2.39	0.45
13:M:65:GLN:HE22	13:M:67:VAL:HB	1.81	0.45
34:h:234:TRP:HA	34:h:237:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:2:190:G:OP1	37:2:603:U:O2'	2.29	0.45
7:G:9:ALA:HB1	7:G:26:LEU:HD13	1.98	0.45
10:J:258:VAL:HG22	10:J:291:PRO:HB2	1.97	0.45
21:U:90:LEU:O	21:U:94:LYS:HG2	2.17	0.45
22:V:117:LYS:NZ	37:2:637:A:OP2	2.39	0.45
32:e:327:ARG:NH2	37:2:473:G:OP2	2.50	0.45
33:f:57:ASP:OD1	33:f:94:SER:HB3	2.16	0.45
34:h:164:ILE:HD12	34:h:201:LEU:HD21	1.97	0.45
23:W:455:GLU:HA	23:W:458:TRP:CD1	2.50	0.45
25:Y:23:ALA:HA	25:Y:28:HIS:HB2	1.98	0.45
28:a:77:VAL:HG11	28:a:104:ALA:HB1	1.97	0.45
33:f:209:GLY:HA2	33:f:212:MET:HE3	1.97	0.45
37:2:228:A:N1	37:2:239:G:O2'	2.39	0.45
2:B:246:LYS:HE2	24:X:453:ASP:HA	1.99	0.45
2:B:288:ARG:CZ	28:a:212:LEU:HB3	2.47	0.45
3:C:167:ARG:NH1	4:D:118:TYR:O	2.49	0.45
8:H:254:ASP:OD1	8:H:254:ASP:N	2.46	0.45
26:Z:55:GLU:OE2	26:Z:119:ARG:NH2	2.48	0.45
33:f:92:LYS:HG2	33:f:143:ILE:HB	1.98	0.45
37:2:1054:U:H2'	37:2:1055:C:C6	2.52	0.45
2:B:191:ILE:HD12	28:a:192:ILE:HD11	1.99	0.45
10:J:262:VAL:HG21	10:J:271:LYS:HB3	1.97	0.45
17:Q:170:GLU:HG2	17:Q:174:LYS:HD2	1.98	0.45
23:W:262:ASP:HB3	23:W:333:VAL:HG21	1.98	0.45
3:C:126:LEU:HD22	3:C:131:ARG:HE	1.81	0.45
6:F:62:GLU:HB2	6:F:79:VAL:HG22	1.98	0.45
27:7:93:VAL:HG22	27:7:105:ILE:HG12	1.98	0.45
27:7:336:TRP:H	27:7:336:TRP:CD1	2.35	0.45
29:b:21:ILE:HD12	37:2:1845:A:C6	2.51	0.45
34:h:327:GLU:O	34:h:331:LYS:HG3	2.16	0.45
37:2:75:C:H2'	37:2:76:G:C8	2.51	0.45
23:W:123:LEU:HD21	23:W:441:TYR:HA	1.99	0.45
34:h:89:LEU:CD1	34:h:108:LEU:HD22	2.47	0.45
37:2:1063:C:H2'	37:2:1064:G:H8	1.81	0.45
37:2:1766:U:H2'	37:2:1767:G:H8	1.82	0.45
37:2:1825:2MG:HM21	37:2:1828:MA6:H2	1.98	0.45
2:B:363:LEU:HD23	24:X:360:TYR:OH	2.16	0.45
32:e:323:TYR:OH	37:2:485:A:N3	2.46	0.45
1:A:128:THR:O	4:D:351:LYS:NZ	2.50	0.45
24:X:373:HIS:O	24:X:377:VAL:HG23	2.17	0.45
27:7:21:PRO:HG3	27:7:110:GLN:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:65:GLN:NE2	13:M:70:ASN:HB2	2.32	0.45
33:f:57:ASP:OD1	33:f:94:SER:CB	2.64	0.45
37:2:291:C:H2'	37:2:292:A:H8	1.82	0.45
37:2:1052:U:H2'	37:2:1053:G:H8	1.82	0.45
3:C:117:LEU:HD11	3:C:126:LEU:HD12	1.99	0.44
3:C:242:LEU:HD23	4:D:207:LEU:HD13	1.98	0.44
8:H:238:LYS:NZ	35:i:305:GLU:OE1	2.43	0.44
11:K:9:ARG:NH2	37:2:874:G:OP2	2.46	0.44
23:W:372:THR:HG22	23:W:374:ARG:H	1.81	0.44
28:a:118:ASP:O	28:a:122:MET:HG2	2.16	0.44
37:2:557:A:H4'	37:2:558:A:H3'	1.98	0.44
2:B:232:PRO:HB2	2:B:333:PHE:HZ	1.82	0.44
34:h:87:LYS:HA	34:h:90:HIS:CD2	2.53	0.44
2:B:38:LEU:HD23	25:Y:59:ILE:HG21	1.99	0.44
2:B:343:LEU:CD2	24:X:376:LEU:CD2	2.94	0.44
23:W:227:VAL:HG13	23:W:237:VAL:HG11	1.99	0.44
27:7:189:SER:HB3	27:7:194:GLU:HB2	1.98	0.44
33:f:104:VAL:C	33:f:106:PRO:HD2	2.42	0.44
34:h:101:ARG:O	37:2:1755:G:O2'	2.35	0.44
37:2:70:U:OP1	37:2:404:C:O2'	2.34	0.44
37:2:839:C:O2'	37:2:840:U:O5'	2.35	0.44
37:2:1669:C:H2'	37:2:1670:A:C8	2.48	0.44
2:B:335:PHE:O	24:X:383:ASN:ND2	2.48	0.44
8:H:307:TYR:OH	37:2:1410:C:O2'	2.29	0.44
37:2:612:U:H2'	37:2:613:C:C6	2.52	0.44
37:2:670:G:H2'	37:2:671:A:C8	2.50	0.44
2:B:13:GLY:HA2	13:M:160:LYS:HZ1	1.81	0.44
7:G:28:PRO:HB3	37:2:649:U:H5	1.83	0.44
17:Q:207:ARG:NH2	37:2:831:G:OP1	2.51	0.44
24:X:337:ASP:OD1	24:X:337:ASP:N	2.49	0.44
28:a:405:GLN:O	28:a:409:MET:HG2	2.18	0.44
29:b:39:SER:HA	29:b:42:ASN:HD22	1.81	0.44
31:d:83:ILE:O	31:d:88:ARG:NH1	2.50	0.44
37:2:411:C:H2'	37:2:412:A:H8	1.83	0.44
37:2:1701:C:H2'	37:2:1702:G:C8	2.53	0.44
2:B:376:VAL:O	2:B:376:VAL:CG1	2.65	0.44
23:W:236:LEU:HB3	23:W:351:VAL:HG12	1.99	0.44
23:W:443:LEU:HD11	23:W:450:ARG:HD2	2.00	0.44
27:7:120:VAL:HG22	27:7:271:VAL:HG11	2.00	0.44
28:a:313:VAL:HG11	28:a:361:ARG:HG2	1.99	0.44
34:h:349:ASP:O	34:h:353:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:2:858:A:H5'	37:2:1070:U:C4	2.52	0.44
3:C:206:ARG:HD3	4:D:90:GLU:HG2	1.99	0.44
9:I:153:TYR:O	37:2:1115:U:O2'	2.23	0.44
23:W:204:LYS:HD3	23:W:205:PRO:HD2	1.98	0.44
23:W:295:LEU:HD21	23:W:310:MET:HB2	2.00	0.44
37:2:1666:C:H2'	37:2:1667:G:C8	2.53	0.44
2:B:243:PHE:CE2	24:X:393:LEU:HD23	2.49	0.44
2:B:434:LYS:HG2	24:X:385:MET:HE2	1.99	0.44
28:a:322:LEU:HD13	28:a:372:ILE:HD11	2.00	0.44
10:J:214:GLY:O	37:2:679:G:N2	2.50	0.44
27:7:273:LEU:HD22	27:7:281:TYR:HB3	1.98	0.44
37:2:215:A:H2'	37:2:216:A:C8	2.53	0.44
37:2:1507:A:H2'	37:2:1508:A:C8	2.52	0.44
2:B:462:ASN:O	2:B:462:ASN:ND2	2.44	0.43
8:H:367:VAL:O	8:H:368:THR:CG2	2.66	0.43
28:a:92:GLU:HG3	28:a:94:ASN:H	1.82	0.43
35:i:281:LYS:HE2	35:i:284:GLY:HA2	2.00	0.43
37:2:354:C:H2'	37:2:355:G:H8	1.83	0.43
2:B:246:LYS:NZ	24:X:457:GLY:O	2.39	0.43
3:C:51:SER:HA	3:C:54:LYS:HE3	2.00	0.43
8:H:219:LYS:O	8:H:222:THR:OG1	2.29	0.43
8:H:367:VAL:C	8:H:368:THR:HG23	2.42	0.43
8:H:412:GLU:OE2	8:H:415:LYS:NZ	2.48	0.43
11:K:31:LEU:HG	11:K:32:GLY:N	2.33	0.43
32:e:188:GLU:HA	32:e:191:ARG:HG2	2.00	0.43
34:h:311:ILE:HA	34:h:314:ILE:HG22	2.00	0.43
37:2:901:A:H2'	37:2:902:A:H8	1.83	0.43
2:B:286:ARG:HH11	2:B:321:ARG:HH22	1.65	0.43
2:B:434:LYS:HA	2:B:434:LYS:HD2	1.85	0.43
4:D:312:ASP:OD1	4:D:344:ARG:NE	2.52	0.43
25:Y:7:LYS:O	25:Y:11:THR:HG23	2.17	0.43
27:7:78:LEU:HD22	27:7:83:ARG:HD2	2.00	0.43
33:f:309:SER:HB3	33:f:368:TRP:CD2	2.53	0.43
35:i:193:PRO:HA	35:i:196:MET:HB2	2.01	0.43
15:O:26:ARG:HE	15:O:26:ARG:HB2	1.66	0.43
23:W:117:GLY:N	23:W:121:ARG:O	2.46	0.43
23:W:207:LYS:NZ	23:W:396:ASP:OD1	2.51	0.43
37:2:547:U:H2'	37:2:548:G:H8	1.83	0.43
37:2:978:C:H2'	37:2:979:A:H8	1.82	0.43
2:B:333:PHE:O	2:B:335:PHE:N	2.49	0.43
8:H:230:ARG:HA	8:H:230:ARG:HD2	1.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:312:ILE:HG22	23:W:324:MET:HE1	2.00	0.43
28:a:209:TRP:O	28:a:210:ASP:HB3	2.18	0.43
32:e:188:GLU:OE2	32:e:191:ARG:NH1	2.50	0.43
37:2:25:U:H2'	37:2:26:U:C6	2.53	0.43
37:2:708:A:H2'	37:2:709:G:C8	2.54	0.43
37:2:718:A:H2	37:2:729:A:H61	1.65	0.43
37:2:997:G:H1	37:2:1029:C:H41	1.66	0.43
34:h:126:PHE:HE2	34:h:166:HIS:HB3	1.84	0.43
37:2:887:G:H2'	37:2:888:G:H8	1.84	0.43
2:B:62:LEU:CD2	2:B:71:ILE:HG23	2.48	0.43
4:D:370:VAL:HG11	37:2:1072:A:C5'	2.48	0.43
10:J:290:ASN:HD21	19:S:34:GLY:HA2	1.83	0.43
28:a:209:TRP:O	28:a:209:TRP:CG	2.71	0.43
37:2:216:A:H2'	37:2:217:A:C8	2.54	0.43
37:2:766:C:H2'	37:2:767:A:H8	1.84	0.43
2:B:13:GLY:HA2	13:M:160:LYS:CE	2.49	0.43
2:B:108:GLY:C	2:B:110:LEU:N	2.77	0.43
2:B:249:MET:SD	28:a:358:GLU:HG2	2.59	0.43
2:B:11:ARG:HH21	2:B:515:PHE:HA	1.83	0.43
2:B:292:PHE:HA	28:a:209:TRP:CE3	2.53	0.43
2:B:392:LEU:HD23	24:X:356:LEU:HD21	2.00	0.43
5:E:10:PHE:HB2	5:E:63:GLN:HB2	2.00	0.43
7:G:111:ASP:OD1	7:G:111:ASP:N	2.48	0.43
37:2:711:A:H2'	37:2:712:A:C8	2.54	0.43
2:B:31:PHE:HZ	28:a:302:GLY:HA3	1.84	0.43
2:B:313:PHE:HD2	2:B:316:LEU:HD22	1.82	0.43
10:J:188:ASN:HD22	17:Q:250:ILE:CG2	2.29	0.43
28:a:178:LYS:O	28:a:182:VAL:HG23	2.19	0.43
33:f:65:LEU:HD11	33:f:155:ILE:HD13	2.00	0.43
4:D:187:LEU:HA	4:D:190:ALA:HB3	2.00	0.42
4:D:295:ASP:OD1	4:D:295:ASP:N	2.50	0.42
18:R:180:LYS:HG2	18:R:181:THR:HG23	2.00	0.42
21:U:7:ASP:OD1	21:U:7:ASP:N	2.47	0.42
27:7:324:HIS:O	27:7:339:TYR:OH	2.33	0.42
37:2:187:C:H2'	37:2:188:G:H8	1.84	0.42
37:2:1412:C:H2'	37:2:1413:A:C8	2.54	0.42
37:2:1822:A:H2'	37:2:1823:G:C8	2.54	0.42
2:B:243:PHE:HE2	24:X:393:LEU:HD23	1.83	0.42
9:I:170:HIS:ND1	9:I:171:VAL:HG22	2.34	0.42
13:M:121:THR:HG22	37:2:1622:A:C8	2.54	0.42
22:V:47:GLU:HG3	22:V:49:TYR:H	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:2:643:U:H2'	37:2:644:G:H8	1.84	0.42
37:2:654:G:H2'	37:2:655:A:C8	2.53	0.42
37:2:820:U:H2'	37:2:821:G:H8	1.84	0.42
7:G:30:SER:HB3	37:2:587:U:H5''	2.01	0.42
33:f:55:ILE:HG13	33:f:92:LYS:HB2	2.01	0.42
37:2:50:A:H2'	37:2:51:U:C6	2.55	0.42
37:2:1664:4OC:HM23	37:2:1664:4OC:H1'	1.88	0.42
1:A:10:LYS:HE3	1:A:187:LEU:HD13	2.01	0.42
2:B:377:MET:HA	2:B:380:ILE:HG12	2.00	0.42
3:C:320:GLU:HG3	32:e:222:LEU:HD12	2.00	0.42
5:E:16:LYS:HG3	22:V:189:LEU:HD13	2.01	0.42
14:N:360:LEU:HA	14:N:363:VAL:HG12	2.02	0.42
28:a:108:ARG:NH2	28:a:117:THR:OG1	2.52	0.42
34:h:169:ARG:HH12	34:h:172:TRP:HH2	1.67	0.42
34:h:203:ASP:O	34:h:207:LYS:HG3	2.19	0.42
37:2:1766:U:H2'	37:2:1767:G:C8	2.55	0.42
3:C:322:ASN:HB2	32:e:222:LEU:HD13	2.01	0.42
37:2:535:G:H2'	37:2:536:G:C8	2.54	0.42
37:2:654:G:H2'	37:2:655:A:H8	1.84	0.42
2:B:284:ARG:HG2	28:a:205:ASP:OD2	2.19	0.42
9:I:142:LYS:NZ	37:2:1416:A:OP1	2.53	0.42
27:7:265:LYS:HE3	37:2:1826:G:H4'	2.01	0.42
2:B:288:ARG:HB3	28:a:213:LEU:HG	2.02	0.42
2:B:427:LEU:HD23	2:B:427:LEU:HA	1.85	0.42
4:D:488:LYS:NZ	37:2:1070:U:H4'	2.35	0.42
14:N:301:LEU:HD23	14:N:301:LEU:HA	1.93	0.42
19:S:71:VAL:HG13	19:S:74:ARG:HH21	1.85	0.42
22:V:155:LEU:O	22:V:159:GLU:HG3	2.20	0.42
24:X:348:MET:HE2	24:X:353:MET:HA	2.02	0.42
37:2:1704:A:H2	37:2:1706:C:H41	1.66	0.42
1:A:2:THR:N	35:i:303:GLU:OE2	2.52	0.42
2:B:147:ARG:NH2	24:X:512:ASP:OD2	2.53	0.42
2:B:254:VAL:HG12	28:a:207:LEU:HD21	2.01	0.42
21:U:52:GLU:OE2	21:U:83:ARG:NE	2.50	0.42
23:W:212:ASP:OD2	23:W:424:ARG:NH1	2.51	0.42
34:h:288:LEU:CD1	34:h:326:LEU:HD21	2.48	0.42
37:2:59:A:N7	37:2:178:U:O2'	2.51	0.42
37:2:613:C:H2'	37:2:614:A:H8	1.84	0.42
2:B:212:PRO:O	2:B:212:PRO:CD	2.67	0.42
34:h:256:PHE:HE2	34:h:279:ARG:HE	1.67	0.42
37:2:48:C:H2'	37:2:49:U:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:2:443:C:O2'	37:2:446:C:OP1	2.37	0.42
37:2:762:A:H3'	37:2:763:A:H8	1.85	0.42
2:B:242:PHE:O	2:B:246:LYS:CB	2.68	0.42
4:D:209:PRO:HB2	35:i:198:MET:HG2	2.01	0.42
6:F:22:GLU:HG3	37:2:1613:U:H4'	2.02	0.42
6:F:34:GLN:HB3	6:F:108:GLU:HG2	2.02	0.42
34:h:331:LYS:HA	34:h:334:VAL:HG22	2.02	0.42
37:2:812:A:OP1	37:2:1835:G:O2'	2.34	0.42
37:2:997:G:H22	37:2:1029:C:H5	1.67	0.42
37:2:1504:G:H2'	37:2:1505:G:H8	1.85	0.42
1:A:116:PHE:HB3	4:D:338:ARG:HG2	2.02	0.41
12:L:45:LEU:HD11	12:L:77:LEU:HD11	2.02	0.41
18:R:35:ILE:HD11	18:R:102:ILE:HB	2.02	0.41
21:U:80:ASP:OD1	21:U:80:ASP:N	2.46	0.41
28:a:336:VAL:HG13	28:a:339:ARG:HB2	2.01	0.41
33:f:317:LEU:HD23	33:f:317:LEU:HA	1.87	0.41
37:2:1080:G:H2'	37:2:1081:G:O4'	2.20	0.41
23:W:190:ILE:HD12	23:W:205:PRO:HB2	2.02	0.41
33:f:253:SER:HB2	35:i:283:TYR:CZ	2.54	0.41
37:2:222:G:H2'	37:2:223:A:H8	1.85	0.41
2:B:288:ARG:NE	28:a:212:LEU:HB3	2.34	0.41
32:e:352:LYS:HD2	32:e:372:VAL:HG22	2.02	0.41
2:B:318:ASN:HA	2:B:321:ARG:HE	1.85	0.41
21:U:90:LEU:HD11	21:U:94:LYS:HE2	2.02	0.41
28:a:380:LYS:HA	28:a:383:GLU:HG2	2.02	0.41
10:J:246:ILE:HD13	10:J:246:ILE:HA	1.96	0.41
33:f:202:LEU:HD21	33:f:317:LEU:HG	2.03	0.41
37:2:49:U:H2'	37:2:50:A:C8	2.56	0.41
37:2:1141:A:H61	37:2:1381:C:H4'	1.85	0.41
37:2:1666:C:H2'	37:2:1667:G:H8	1.84	0.41
2:B:343:LEU:CD2	24:X:376:LEU:HD23	2.48	0.41
3:C:139:VAL:HG12	3:C:141:ILE:H	1.86	0.41
4:D:148:SER:OG	4:D:149:ASP:N	2.52	0.41
13:M:76:ARG:HD3	13:M:122:ARG:HG3	2.01	0.41
15:O:85:PRO:HA	15:O:86:PRO:HD3	1.96	0.41
18:R:28:TYR:HA	18:R:106:VAL:HG11	2.03	0.41
33:f:389:THR:HG22	33:f:397:GLU:CB	2.41	0.41
37:2:1576:C:H2'	37:2:1577:U:C6	2.55	0.41
13:M:65:GLN:NE2	13:M:67:VAL:O	2.53	0.41
13:M:87:ARG:NH2	13:M:118:SER:OG	2.51	0.41
34:h:353:VAL:HG12	34:h:357:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:2:192:G:H2'	37:2:193:A:C8	2.55	0.41
37:2:590:A:H2'	37:2:591:U:H6	1.86	0.41
37:2:1381:C:O2'	37:2:1382:C:O4'	2.35	0.41
2:B:356:ARG:NH1	24:X:368:LEU:O	2.53	0.41
28:a:344:LYS:HG3	37:2:1403:U:H4'	2.02	0.41
33:f:319:SER:HA	33:f:334:ARG:NH1	2.36	0.41
3:C:297:PHE:HE2	32:e:153:PHE:HZ	1.69	0.41
9:I:134:ILE:HD12	9:I:188:LEU:HD13	2.01	0.41
9:I:157:PRO:HG3	37:2:1413:A:H4'	2.03	0.41
10:J:216:VAL:O	37:2:680:U:O2'	2.35	0.41
18:R:35:ILE:HG13	18:R:38:LEU:HD21	2.02	0.41
21:U:42:ASN:O	21:U:44:ASN:N	2.53	0.41
28:a:213:LEU:HD23	28:a:213:LEU:HA	1.86	0.41
31:d:92:LEU:HD13	37:2:478:U:H5''	2.03	0.41
32:e:239:ASP:OD1	32:e:239:ASP:N	2.53	0.41
34:h:225:PHE:HA	34:h:228:CYS:SG	2.61	0.41
34:h:263:ALA:O	34:h:266:ARG:HG2	2.21	0.41
37:2:765:G:H4'	37:2:1822:A:H4'	2.03	0.41
37:2:1475:U:H5'	37:2:1476:A:C8	2.56	0.41
37:2:1481:C:H2'	37:2:1482:U:C6	2.55	0.41
6:F:11:LEU:HD12	6:F:89:ILE:HD11	2.03	0.41
7:G:104:THR:HG22	37:2:638:A:N3	2.35	0.41
10:J:202:ARG:NH2	37:2:688:U:OP2	2.54	0.41
25:Y:63:ASP:HB3	25:Y:66:VAL:HG22	2.04	0.41
26:Z:86:LEU:HD22	34:h:137:LEU:HD23	2.03	0.41
27:7:200:ALA:HB1	27:7:204:ARG:HH12	1.86	0.41
32:e:164:MET:HE2	32:e:164:MET:HB2	1.91	0.41
34:h:250:LYS:HE3	34:h:250:LYS:HB3	1.81	0.41
34:h:302:HIS:HE1	34:h:356:SER:HB2	1.83	0.41
37:2:82:C:O2'	37:2:83:U:O5'	2.35	0.41
37:2:1504:G:H2'	37:2:1505:G:C8	2.55	0.41
10:J:284:ASN:HD21	29:b:46:LEU:HD13	1.86	0.40
11:K:64:PHE:HE2	37:2:1674:C:H5'	1.86	0.40
21:U:24:PRO:HG2	21:U:27:LEU:HB2	2.03	0.40
23:W:281:ARG:HH21	23:W:349:VAL:HG11	1.86	0.40
26:Z:60:LEU:HD12	26:Z:67:TYR:HD2	1.86	0.40
27:7:200:ALA:HB2	27:7:225:LEU:HD22	2.03	0.40
35:i:201:PHE:O	35:i:205:ILE:HG12	2.21	0.40
37:2:573:G:O2'	37:2:817:G:H5'	2.22	0.40
37:2:993:G:H2'	37:2:994:A:C8	2.57	0.40
2:B:460:LEU:HD13	2:B:533:LEU:HD21	2.00	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:119:ARG:HA	12:L:119:ARG:HD2	1.85	0.40
35:i:328:LEU:O	35:i:365:HIS:NE2	2.54	0.40
1:A:157:VAL:HG22	1:A:174:TYR:HB2	2.04	0.40
2:B:67:LYS:HB3	24:X:385:MET:HE3	2.03	0.40
2:B:397:ASP:OD1	24:X:366:ARG:NH2	2.54	0.40
2:B:401:GLU:OE2	24:X:366:ARG:NH2	2.51	0.40
6:F:5:ASP:OD1	6:F:5:ASP:N	2.48	0.40
6:F:146:ARG:HH21	29:b:31:LYS:HB3	1.87	0.40
10:J:250:VAL:HG13	10:J:255:LEU:HB2	2.03	0.40
23:W:221:ILE:HG12	23:W:225:MET:HE2	2.03	0.40
24:X:401:PRO:HG3	28:a:361:ARG:CD	2.51	0.40
32:e:256:ASP:OD1	32:e:256:ASP:N	2.55	0.40
37:2:817:G:H2'	37:2:818:A:C8	2.56	0.40
2:B:204:THR:HG23	2:B:207:PHE:H	1.86	0.40
4:D:475:SER:O	37:2:15:A:O2'	2.38	0.40
6:F:137:SER:HA	29:b:41:LEU:HD22	2.03	0.40
10:J:272:ARG:HG3	19:S:40:LEU:HD13	2.02	0.40
22:V:189:LEU:O	22:V:192:SER:OG	2.36	0.40
23:W:293:ILE:HG13	23:W:338:ARG:HH11	1.87	0.40
23:W:457:ASN:HB3	23:W:479:MET:HG3	2.03	0.40
33:f:39:VAL:HG12	33:f:39:VAL:O	2.21	0.40
34:h:296:LYS:HE2	34:h:333:LEU:HD21	2.03	0.40
36:k:12:ASN:O	36:k:15:LYS:HG3	2.21	0.40
37:2:1387:C:O2'	37:2:1388:A:O4'	2.35	0.40
37:2:1575:U:H2'	37:2:1576:C:C6	2.56	0.40
37:2:1697:G:H2'	37:2:1698:C:C6	2.57	0.40
4:D:114:ASP:N	4:D:114:ASP:OD1	2.54	0.40
6:F:7:GLU:HG3	6:F:85:GLN:HE22	1.87	0.40
10:J:272:ARG:O	10:J:276:VAL:HG23	2.21	0.40
14:N:316:PRO:HA	14:N:319:MET:HE2	2.03	0.40
16:P:36:ARG:NH1	37:2:257:G:OP1	2.50	0.40
37:2:369:G:H2'	37:2:370:G:C8	2.57	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	202/212 (95%)	198 (98%)	4 (2%)	0	100	100
2	B	457/554 (82%)	430 (94%)	24 (5%)	3 (1%)	18	21
3	C	329/362 (91%)	324 (98%)	5 (2%)	0	100	100
4	D	413/501 (82%)	396 (96%)	17 (4%)	0	100	100
5	E	99/138 (72%)	99 (100%)	0	0	100	100
6	F	146/157 (93%)	140 (96%)	6 (4%)	0	100	100
7	G	126/129 (98%)	124 (98%)	2 (2%)	0	100	100
8	H	207/383 (54%)	198 (96%)	8 (4%)	1 (0%)	24	29
9	I	111/228 (49%)	108 (97%)	3 (3%)	0	100	100
10	J	125/304 (41%)	119 (95%)	6 (5%)	0	100	100
11	K	122/125 (98%)	120 (98%)	2 (2%)	0	100	100
12	L	107/154 (70%)	104 (97%)	3 (3%)	0	100	100
13	M	99/155 (64%)	99 (100%)	0	0	100	100
14	N	114/414 (28%)	114 (100%)	0	0	100	100
15	O	108/136 (79%)	106 (98%)	2 (2%)	0	100	100
16	P	89/110 (81%)	87 (98%)	2 (2%)	0	100	100
17	Q	88/237 (37%)	87 (99%)	1 (1%)	0	100	100
18	R	162/212 (76%)	157 (97%)	5 (3%)	0	100	100
19	S	73/100 (73%)	73 (100%)	0	0	100	100
20	T	48/94 (51%)	46 (96%)	2 (4%)	0	100	100
21	U	125/192 (65%)	121 (97%)	4 (3%)	0	100	100
22	V	162/193 (84%)	158 (98%)	4 (2%)	0	100	100
23	W	376/483 (78%)	371 (99%)	5 (1%)	0	100	100
24	X	202/496 (41%)	199 (98%)	3 (2%)	0	100	100
25	Y	96/102 (94%)	95 (99%)	0	1 (1%)	12	13
26	Z	79/153 (52%)	78 (99%)	1 (1%)	0	100	100
27	7	357/496 (72%)	340 (95%)	16 (4%)	1 (0%)	36	44
28	a	311/424 (73%)	305 (98%)	5 (2%)	1 (0%)	36	44
29	b	71/80 (89%)	63 (89%)	8 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	c	24/128 (19%)	24 (100%)	0	0	100	100
31	d	76/110 (69%)	76 (100%)	0	0	100	100
32	e	244/383 (64%)	234 (96%)	10 (4%)	0	100	100
33	f	373/410 (91%)	364 (98%)	9 (2%)	0	100	100
34	h	308/384 (80%)	297 (96%)	11 (4%)	0	100	100
35	i	302/725 (42%)	295 (98%)	7 (2%)	0	100	100
36	k	20/153 (13%)	18 (90%)	2 (10%)	0	100	100
All	All	6351/9617 (66%)	6167 (97%)	177 (3%)	7 (0%)	49	59

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
28	a	210	ASP
2	B	481	ARG
8	H	225	ILE
25	Y	95	ARG
2	B	104	ALA
27	7	368	VAL
2	B	109	CYS

### 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	177/182 (97%)	177 (100%)	0	100	100
2	B	421/492 (86%)	420 (100%)	1 (0%)	87	93
3	C	312/343 (91%)	312 (100%)	0	100	100
4	D	370/444 (83%)	370 (100%)	0	100	100
5	E	90/126 (71%)	90 (100%)	0	100	100
6	F	124/124 (100%)	124 (100%)	0	100	100
7	G	112/113 (99%)	112 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	174/320 (54%)	174 (100%)	0	100	100
9	I	104/197 (53%)	104 (100%)	0	100	100
10	J	109/256 (43%)	109 (100%)	0	100	100
11	K	106/107 (99%)	106 (100%)	0	100	100
12	L	92/128 (72%)	92 (100%)	0	100	100
13	M	90/137 (66%)	90 (100%)	0	100	100
14	N	107/362 (30%)	107 (100%)	0	100	100
15	O	93/117 (80%)	93 (100%)	0	100	100
16	P	78/95 (82%)	78 (100%)	0	100	100
17	Q	75/203 (37%)	75 (100%)	0	100	100
18	R	141/180 (78%)	141 (100%)	0	100	100
19	S	68/90 (76%)	68 (100%)	0	100	100
20	T	44/79 (56%)	44 (100%)	0	100	100
21	U	109/170 (64%)	108 (99%)	1 (1%)	70	82
22	V	147/173 (85%)	147 (100%)	0	100	100
23	W	328/410 (80%)	328 (100%)	0	100	100
24	X	174/395 (44%)	174 (100%)	0	100	100
25	Y	84/86 (98%)	84 (100%)	0	100	100
26	Z	66/119 (56%)	66 (100%)	0	100	100
27	7	321/437 (74%)	321 (100%)	0	100	100
28	a	252/375 (67%)	252 (100%)	0	100	100
29	b	66/71 (93%)	66 (100%)	0	100	100
30	c	25/116 (22%)	25 (100%)	0	100	100
31	d	65/93 (70%)	65 (100%)	0	100	100
32	e	226/339 (67%)	226 (100%)	0	100	100
33	f	319/351 (91%)	319 (100%)	0	100	100
34	h	271/337 (80%)	271 (100%)	0	100	100
35	i	272/629 (43%)	272 (100%)	0	100	100
36	k	17/109 (16%)	17 (100%)	0	100	100
All	All	5629/8305 (68%)	5627 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	462	ASN
21	U	42	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	66	ASN
1	A	163	ASN
2	B	64	HIS
2	B	240	GLN
2	B	244	ASN
2	B	258	ASN
2	B	282	GLN
2	B	351	ASN
2	B	361	ASN
2	B	516	ASN
3	C	70	GLN
3	C	88	HIS
3	C	102	ASN
3	C	125	GLN
3	C	155	GLN
3	C	255	ASN
4	D	168	ASN
4	D	179	GLN
4	D	234	GLN
5	E	80	HIS
6	F	85	GLN
6	F	131	ASN
6	F	139	ASN
8	H	364	ASN
9	I	213	GLN
10	J	284	ASN
11	K	10	HIS
13	M	65	GLN
16	P	27	ASN
19	S	59	GLN
19	S	63	HIS
21	U	42	ASN
23	W	307	GLN
24	X	520	GLN
24	X	521	ASN
25	Y	28	HIS

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Mol	Chain	Res	Type
25	Y	93	HIS
28	a	126	GLN
28	a	158	ASN
29	b	48	ASN
32	e	193	HIS
33	f	133	GLN
33	f	220	HIS
33	f	318	GLN
34	h	217	GLN
34	h	302	HIS
36	k	2	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
37	2	1555/1560 (99%)	261 (16%)	10 (0%)

All (261) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
37	2	4	A
37	2	5	U
37	2	12	A
37	2	17	G
37	2	30	G
37	2	40	A
37	2	47	G
37	2	55	C
37	2	56	U
37	2	59	A
37	2	60	C
37	2	76	G
37	2	78	U
37	2	79	G
37	2	82	C
37	2	83	U
37	2	150	A
37	2	151	A
37	2	152	G
37	2	154	G
37	2	156	U

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Mol	Chain	Res	Type
37	2	157	G
37	2	161	A
37	2	162	C
37	2	163	A
37	2	164	A
37	2	172	A
37	2	183	A
37	2	184	A
37	2	185	G
37	2	194	A
37	2	195	U
37	2	203	A
37	2	206	G
37	2	208	U
37	2	214	U
37	2	215	A
37	2	228	A
37	2	233	G
37	2	236	A
37	2	245	U
37	2	246	G
37	2	264	U
37	2	266	G
37	2	270	G
37	2	285	G
37	2	286	C
37	2	288	G
37	2	299	U
37	2	308	G
37	2	317	U
37	2	318	U
37	2	325	A
37	2	340	A
37	2	347	C
37	2	351	G
37	2	363	A
37	2	364	C
37	2	365	G
37	2	366	G
37	2	371	C
37	2	373	G
37	2	386	U

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Mol	Chain	Res	Type
37	2	391	C
37	2	403	G
37	2	408	A
37	2	416	A
37	2	420	U
37	2	421	G
37	2	425	G
37	2	430	A
37	2	432	G
37	2	440	A
37	2	441	U
37	2	442	U
37	2	443	C
37	2	444	C
37	2	450	U
37	2	459	U
37	2	468	U
37	2	469	G
37	2	470	C
37	2	471	G
37	2	492	G
37	2	493	A
37	2	494	A
37	2	495	G
37	2	507	A
37	2	509	C
37	2	516	C
37	2	519	G
37	2	522	G
37	2	530	A
37	2	545	A
37	2	557	A
37	2	560	G
37	2	562	C
37	2	566	G
37	2	570	A
37	2	571	A
37	2	573	G
37	2	574	G
37	2	575	G
37	2	593	G
37	2	629	G

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Mol	Chain	Res	Type
37	2	661	A
37	2	683	A
37	2	684	G
37	2	687	G
37	2	699	G
37	2	717	A
37	2	718	A
37	2	720	A
37	2	745	A
37	2	751	G
37	2	762	A
37	2	773	A
37	2	789	U
37	2	790	A
37	2	805	G
37	2	811	A
37	2	813	C
37	2	817	G
37	2	825	G
37	2	832	G
37	2	836	A
37	2	837	U
37	2	838	U
37	2	839	C
37	2	840	U
37	2	846	G
37	2	865	A
37	2	866	A
37	2	878	G
37	2	893	A
37	2	895	G
37	2	907	A
37	2	919	G
37	2	927	C
37	2	928	A
37	2	932	G
37	2	953	U
37	2	962	A
37	2	964	G
37	2	968	A
37	2	969	G
37	2	970	A

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Mol	Chain	Res	Type
37	2	975	U
37	2	982	C
37	2	986	G
37	2	998	A
37	2	999	G
37	2	1007	A
37	2	1012	U
37	2	1029	C
37	2	1030	U
37	2	1037	C
37	2	1057	U
37	2	1078	U
37	2	1081	G
37	2	1082	U
37	2	1086	G
37	2	1093	A
37	2	1116	G
37	2	1117	U
37	2	1118	U
37	2	1122	C
37	2	1123	A
37	2	1125	A
37	2	1127	A
37	2	1128	U
37	2	1135	A
37	2	1137	G
37	2	1138	G
37	2	1139	A
37	2	1140	G
37	2	1380	U
37	2	1381	C
37	2	1382	C
37	2	1386	A
37	2	1387	C
37	2	1389	A
37	2	1391	C
37	2	1392	A
37	2	1398	G
37	2	1399	U
37	2	1402	G
37	2	1407	G
37	2	1420	A

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Mol	Chain	Res	Type
37	2	1422	U
37	2	1429	G
37	2	1430	A
37	2	1432	A
37	2	1459	A
37	2	1460	A
37	2	1475	U
37	2	1476	A
37	2	1490	A
37	2	1491	C
37	2	1501	A
37	2	1504	G
37	2	1511	A
37	2	1516	G
37	2	1521	G
37	2	1523	A
37	2	1542	A
37	2	1543	A
37	2	1562	G
37	2	1582	C
37	2	1608	A
37	2	1615	G
37	2	1625	A
37	2	1626	U
37	2	1643	A
37	2	1651	C
37	2	1652	C
37	2	1660	A
37	2	1702	G
37	2	1703	G
37	2	1706	C
37	2	1707	A
37	2	1714	A
37	2	1717	C
37	2	1722	C
37	2	1723	U
37	2	1725	C
37	2	1727	G
37	2	1728	U
37	2	1731	A
37	2	1732	A
37	2	1735	C

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Mol	Chain	Res	Type
37	2	1736	U
37	2	1740	C
37	2	1742	C
37	2	1743	A
37	2	1744	C
37	2	1745	A
37	2	1746	A
37	2	1750	C
37	2	1751	U
37	2	1752	U
37	2	1760	U
37	2	1762	U
37	2	1763	U
37	2	1764	A
37	2	1766	U
37	2	1768	A
37	2	1771	C
37	2	1774	A
37	2	1795	G
37	2	1801	A
37	2	1802	A
37	2	1806	G
37	2	1812	A
37	2	1815	U
37	2	1825	2MG
37	2	1826	G
37	2	1827	MA6
37	2	1838	G
37	2	1839	G
37	2	1848	C

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
37	2	317	U
37	2	491	G
37	2	493	A
37	2	573	G
37	2	998	A
37	2	1117	U
37	2	1701	C
37	2	1705	C

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Mol	Chain	Res	Type
37	2	1706	C
37	2	1726	U

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

6 non-standard protein/DNA/RNA residues are 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	$\# Z  > 2$
37	UR3	2	1807	37	19,22,23	2.86	8 (42%)	26,32,35	1.63	3 (11%)
37	MA6	2	1827	37	23,26,27	1.67	5 (21%)	33,38,41	3.45	12 (36%)
37	G7M	2	525	37	23,26,27	2.31	7 (30%)	34,39,42	3.11	10 (29%)
37	4OC	2	1664	37	20,23,24	3.43	8 (40%)	25,32,35	0.90	1 (4%)
37	2MG	2	1825	37	23,26,27	2.95	7 (30%)	33,38,41	3.23	14 (42%)
37	MA6	2	1828	37	23,26,27	1.62	5 (21%)	33,38,41	3.52	11 (33%)

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
37	UR3	2	1807	37	-	2/7/25/26	0/2/2/2
37	MA6	2	1827	37	-	7/11/29/30	0/3/3/3
37	G7M	2	525	37	-	3/7/25/26	0/3/3/3
37	4OC	2	1664	37	-	0/9/29/30	0/2/2/2
37	2MG	2	1825	37	-	2/9/27/28	0/3/3/3
37	MA6	2	1828	37	-	6/11/29/30	0/3/3/3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	2	1825	2MG	C2-N3	7.83	1.46	1.32
37	2	1825	2MG	C2-N2	7.79	1.49	1.33
37	2	1664	4OC	C4-N3	7.78	1.45	1.32
37	2	1807	UR3	C2-N1	7.57	1.49	1.38
37	2	525	G7M	C4-N3	6.80	1.49	1.34
37	2	1664	4OC	C2-N3	6.75	1.49	1.36
37	2	1664	4OC	C6-C5	6.59	1.50	1.35
37	2	1807	UR3	C6-C5	6.29	1.49	1.35
37	2	1825	2MG	C4-N3	5.95	1.47	1.34
37	2	1664	4OC	C4-N4	5.93	1.48	1.36
37	2	1828	MA6	C6-N6	5.11	1.51	1.36
37	2	1827	MA6	C6-N6	5.07	1.50	1.36
37	2	1807	UR3	C2-N3	5.06	1.49	1.39
37	2	1825	2MG	C2-N1	4.45	1.43	1.36
37	2	525	G7M	C2-N2	4.29	1.44	1.34
37	2	1664	4OC	C2-N1	4.18	1.48	1.40
37	2	525	G7M	C2-N3	4.08	1.43	1.33
37	2	525	G7M	C5-N7	-3.80	1.34	1.39
37	2	1664	4OC	C5-C4	3.79	1.49	1.41
37	2	1664	4OC	C6-N1	3.30	1.46	1.38
37	2	1807	UR3	C6-N1	3.03	1.45	1.38
37	2	525	G7M	C5-C6	2.79	1.51	1.43
37	2	1828	MA6	C5-N7	-2.74	1.34	1.39
37	2	1827	MA6	C5-N7	-2.67	1.34	1.39
37	2	525	G7M	C6-N1	2.65	1.43	1.38
37	2	1827	MA6	C10-N6	2.64	1.51	1.45
37	2	1825	2MG	C5-C6	2.63	1.54	1.44
37	2	1807	UR3	C4-N3	2.53	1.45	1.40
37	2	1827	MA6	C5-C4	-2.52	1.34	1.39
37	2	1828	MA6	C10-N6	2.51	1.51	1.45
37	2	1664	4OC	O2-C2	-2.48	1.19	1.23
37	2	1825	2MG	C6-N1	2.42	1.43	1.38
37	2	525	G7M	C2-N1	2.41	1.43	1.37
37	2	1807	UR3	O4-C4	-2.39	1.18	1.23
37	2	1828	MA6	C5-C4	-2.38	1.34	1.39
37	2	1807	UR3	C5-C4	2.35	1.49	1.43
37	2	1807	UR3	O2-C2	-2.24	1.18	1.22
37	2	1827	MA6	C8-N9	-2.18	1.33	1.37
37	2	1828	MA6	C8-N9	-2.11	1.33	1.37
37	2	1825	2MG	C5-N7	-2.08	1.34	1.39

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	2	1828	MA6	N1-C6-N6	-12.89	101.15	116.86
37	2	1827	MA6	N1-C6-N6	-12.56	101.55	116.86
37	2	525	G7M	CN7-N7-C5	9.39	138.50	126.80
37	2	1828	MA6	C5-C6-N6	8.48	138.75	125.33
37	2	1827	MA6	C5-C6-N6	8.25	138.38	125.33
37	2	1825	2MG	C1'-N9-C4	8.09	150.37	126.49
37	2	1825	2MG	C1'-N9-C8	-7.97	104.09	126.73
37	2	525	G7M	CN7-N7-C8	-7.29	113.74	124.79
37	2	525	G7M	C1'-N9-C4	7.19	147.74	126.49
37	2	1825	2MG	N1-C2-N2	6.42	123.12	116.56
37	2	1825	2MG	C2-N3-C4	6.41	120.02	112.00
37	2	525	G7M	C1'-N9-C8	-6.40	105.14	126.74
37	2	1828	MA6	C5-C4-N3	-5.95	118.52	126.72
37	2	1807	UR3	C4-N3-C2	-5.82	119.90	124.58
37	2	1827	MA6	N1-C2-N3	-5.78	119.83	128.58
37	2	1828	MA6	N1-C2-N3	-5.40	120.40	128.58
37	2	1825	2MG	C5-C4-N3	-5.29	119.98	128.39
37	2	1827	MA6	C5-C4-N3	-5.26	119.47	126.72
37	2	1825	2MG	C2-N1-C6	-4.98	118.53	124.55
37	2	1825	2MG	CM2-N2-C2	-4.73	113.49	123.65
37	2	525	G7M	C2-N3-C4	4.52	120.08	112.30
37	2	1827	MA6	N9-C8-N7	-4.52	107.53	113.94
37	2	1828	MA6	C4-C5-C6	4.40	120.45	115.91
37	2	525	G7M	C5-C4-N3	-4.27	120.09	128.15
37	2	1828	MA6	N3-C4-N9	4.21	134.32	127.17
37	2	1828	MA6	N9-C8-N7	-4.07	108.16	113.94
37	2	525	G7M	C5-C6-N1	3.94	119.99	111.84
37	2	1827	MA6	C4-C5-C6	3.92	119.97	115.91
37	2	1828	MA6	C2-N3-C4	3.73	120.93	111.83
37	2	1825	2MG	N2-C2-N3	-3.72	115.78	120.51
37	2	1827	MA6	N3-C4-N9	3.70	133.46	127.17
37	2	1807	UR3	C5-C4-N3	3.66	119.86	115.04
37	2	1827	MA6	C2-N3-C4	3.55	120.50	111.83
37	2	525	G7M	O6-C6-C5	-3.43	120.34	128.01
37	2	1827	MA6	C2-N1-C6	3.41	120.16	111.83
37	2	1828	MA6	C2-N1-C6	3.17	119.58	111.83
37	2	1827	MA6	C5-N7-C8	3.08	108.29	103.45
37	2	525	G7M	C2-N1-C6	-3.06	119.56	125.11
37	2	1828	MA6	C5-N7-C8	2.98	108.13	103.45
37	2	1827	MA6	C4-N9-C8	2.96	108.85	105.74
37	2	1825	2MG	C5-C6-N1	2.77	120.29	113.25
37	2	525	G7M	N9-C4-N3	2.51	130.98	125.95
37	2	1825	2MG	O6-C6-C5	-2.49	119.95	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	2	1664	4OC	C6-C5-C4	2.48	119.99	117.00
37	2	1825	2MG	C5-C4-N9	2.46	110.07	105.66
37	2	1828	MA6	C4-N9-C8	2.33	108.18	105.74
37	2	1807	UR3	C6-N1-C2	-2.17	120.02	121.80
37	2	1825	2MG	N9-C8-N7	-2.11	109.49	113.40
37	2	1825	2MG	C4-C5-N7	-2.05	107.42	110.67
37	2	1827	MA6	C4-C5-N7	-2.03	108.26	110.58
37	2	1825	2MG	N9-C4-N3	2.00	129.96	125.95

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
37	2	1825	2MG	O4'-C4'-C5'-O5'
37	2	1827	MA6	O4'-C4'-C5'-O5'
37	2	1827	MA6	C3'-C4'-C5'-O5'
37	2	1827	MA6	C5-C6-N6-C10
37	2	1828	MA6	O4'-C1'-N9-C4
37	2	1828	MA6	O4'-C1'-N9-C8
37	2	1828	MA6	C5-C6-N6-C9
37	2	1807	UR3	O4'-C4'-C5'-O5'
37	2	1825	2MG	C3'-C4'-C5'-O5'
37	2	1828	MA6	N1-C6-N6-C9
37	2	1827	MA6	N1-C6-N6-C10
37	2	1807	UR3	C3'-C4'-C5'-O5'
37	2	1828	MA6	C5-C6-N6-C10
37	2	525	G7M	C3'-C4'-C5'-O5'
37	2	1828	MA6	C3'-C4'-C5'-O5'
37	2	1827	MA6	O4'-C1'-N9-C4
37	2	525	G7M	C4'-C5'-O5'-P
37	2	1827	MA6	O4'-C1'-N9-C8
37	2	1827	MA6	C5-C6-N6-C9
37	2	525	G7M	O4'-C4'-C5'-O5'

There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	2	1827	MA6	1	0
37	2	1664	4OC	1	0
37	2	1825	2MG	1	0

*Continued on next page...*

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	2	1828	MA6	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 98 ligands modelled in this entry, 96 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
40	ATP	W	501	39	32,33,33	0.38	0	48,52,52	0.30	0
42	GTP	7	602	39	33,34,34	0.93	1 (3%)	50,54,54	1.58	8 (16%)

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
40	ATP	W	501	39	-	1/22/38/38	0/3/3/3
42	GTP	7	602	39	-	5/22/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	7	602	GTP	C2-N3	2.06	1.38	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	7	602	GTP	C5-C4-N3	-4.82	120.72	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	7	602	GTP	C2-N3-C4	4.52	120.09	112.30
42	7	602	GTP	N9-C4-N3	2.94	131.84	125.95
42	7	602	GTP	C2-N1-C6	-2.83	119.98	125.11
42	7	602	GTP	N9-C8-N7	-2.67	108.45	113.40
42	7	602	GTP	C8-N7-C5	2.52	108.75	104.26
42	7	602	GTP	C5-C6-N1	2.44	119.46	113.25
42	7	602	GTP	O6-C6-C5	-2.30	120.45	126.53

There are no chirality outliers.

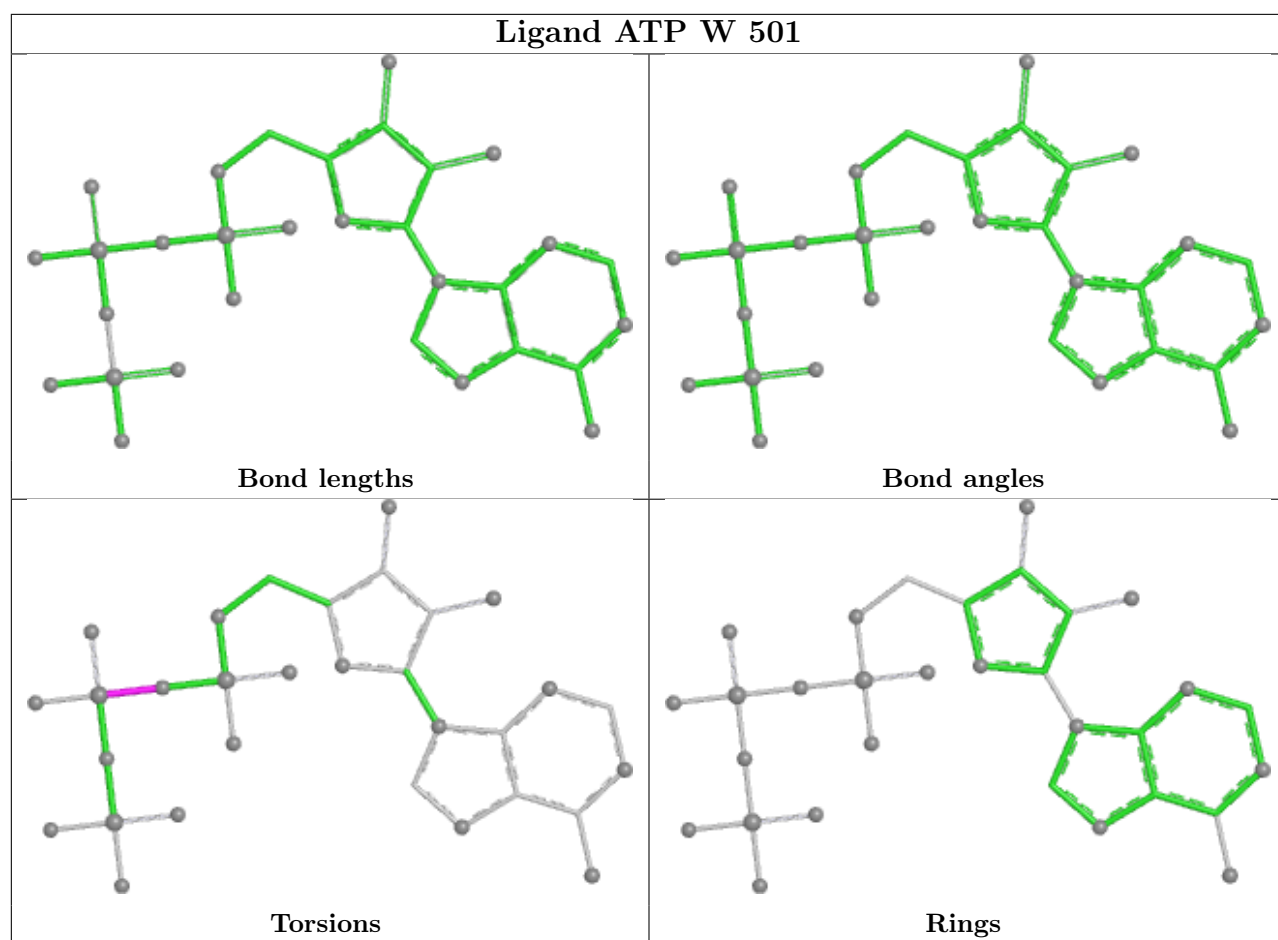
All (6) torsion outliers are listed below:

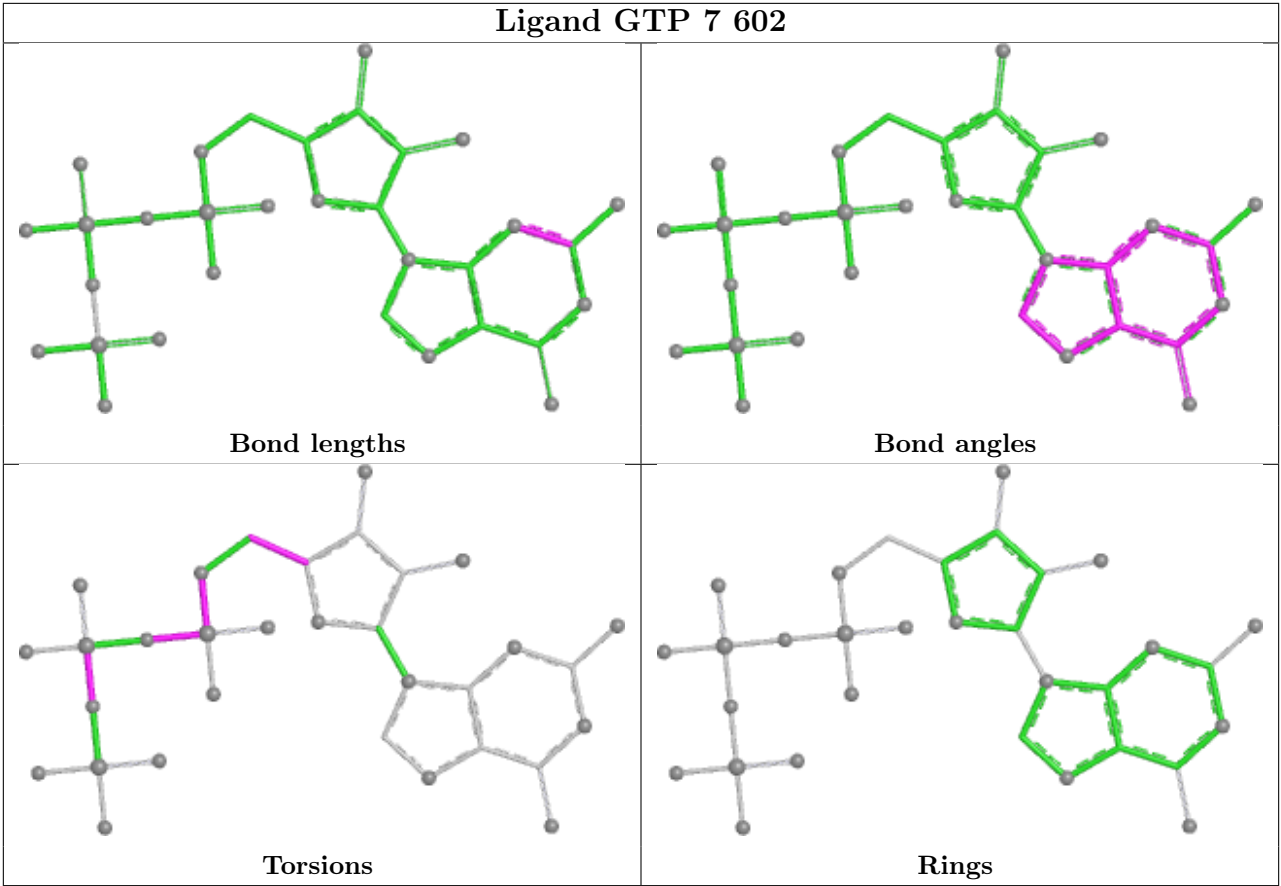
Mol	Chain	Res	Type	Atoms
42	7	602	GTP	O4'-C4'-C5'-O5'
40	W	501	ATP	PA-O3A-PB-O1B
42	7	602	GTP	PB-O3A-PA-O2A
42	7	602	GTP	C5'-O5'-PA-O1A
42	7	602	GTP	PG-O3B-PB-O2B
42	7	602	GTP	PG-O3B-PB-O1B

There are no ring outliers.

No monomer is involved in short contacts.

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





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
37	2	6

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	1142:A	O3'	1379:C	P	16.35
1	2	137:A	O3'	142:U	P	15.19
1	2	84:A	O3'	129:A	P	11.35
1	2	1842:U	O3'	1845:A	P	7.73
1	2	921:G	O3'	922:G	P	1.83
1	2	1650:C	O3'	1651:C	P	1.28

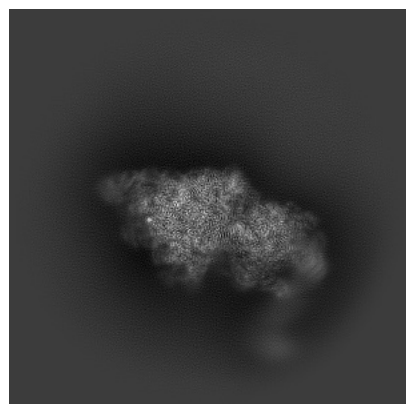
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50014. These allow visual inspection of the internal detail of the map and identification of artifacts.

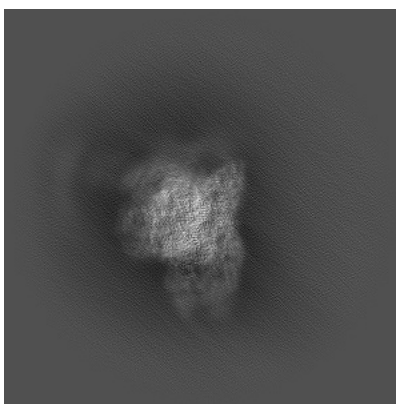
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

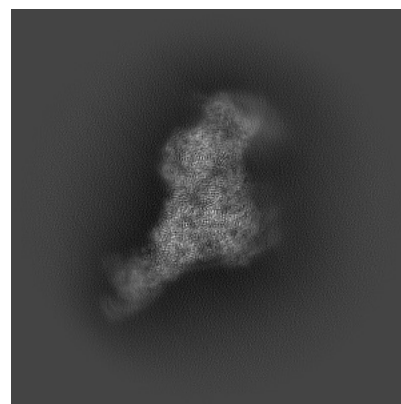
#### 6.1.1 Primary map



X

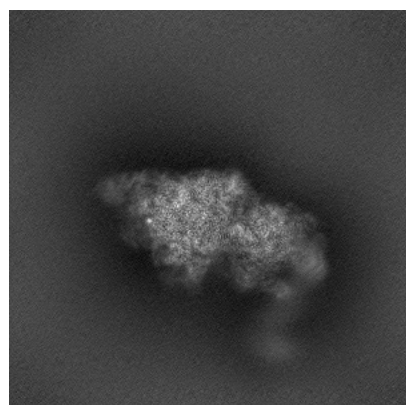


Y

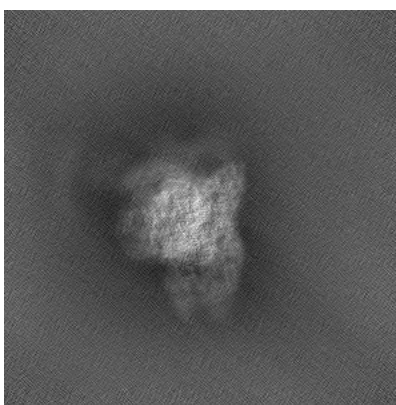


Z

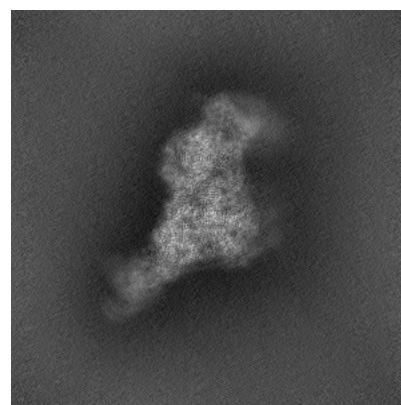
#### 6.1.2 Raw map



X



Y



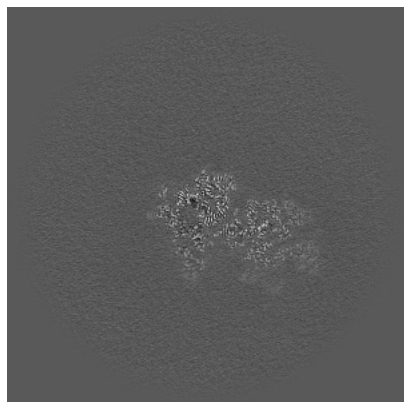
Z

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

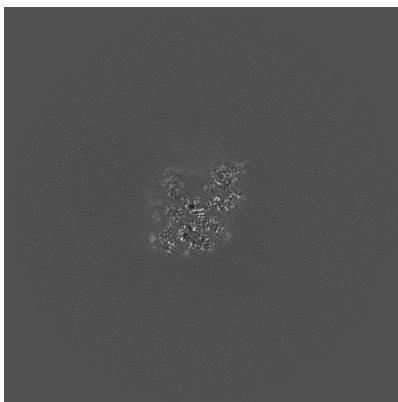


## 6.2 Central slices [i](#)

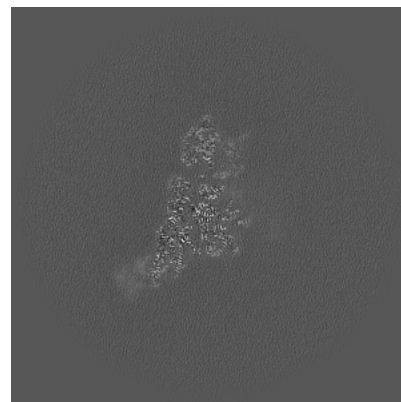
### 6.2.1 Primary map



X Index: 294

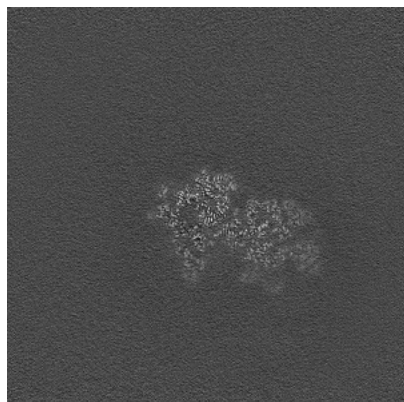


Y Index: 294

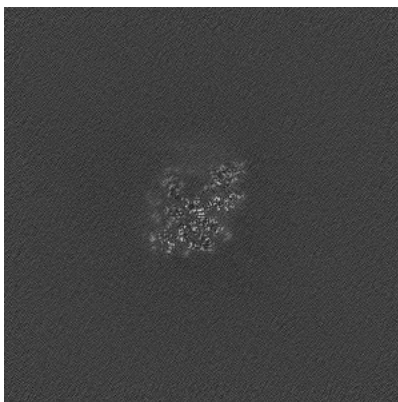


Z Index: 294

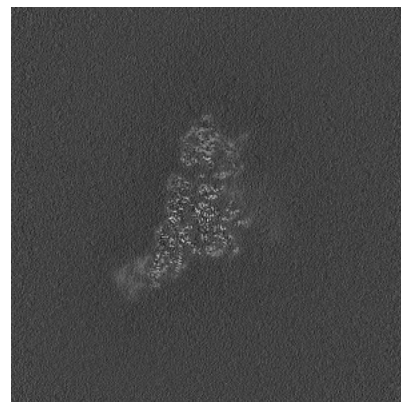
### 6.2.2 Raw map



X Index: 294



Y Index: 294

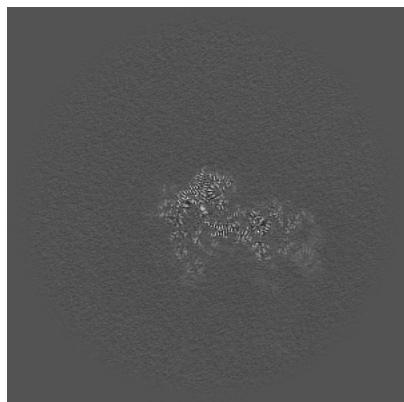


Z Index: 294

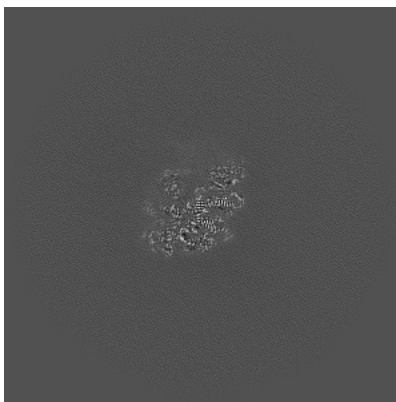
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

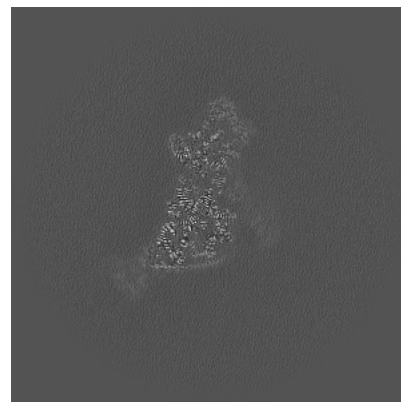
### 6.3.1 Primary map



X Index: 300

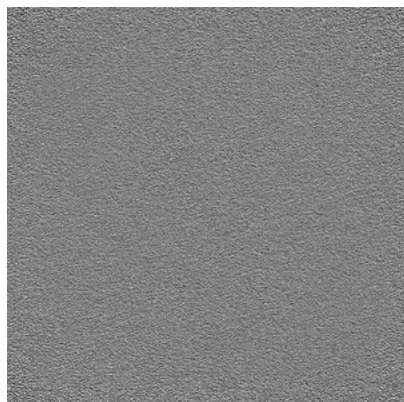


Y Index: 290

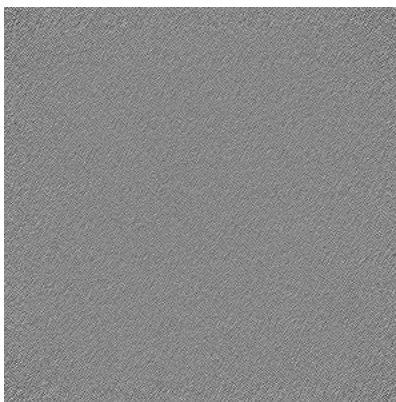


Z Index: 280

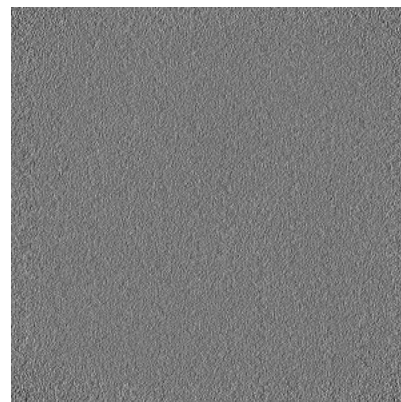
### 6.3.2 Raw map



X Index: 0



Y Index: 0



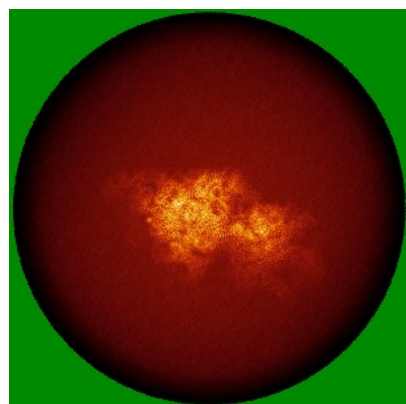
Z Index: 0

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

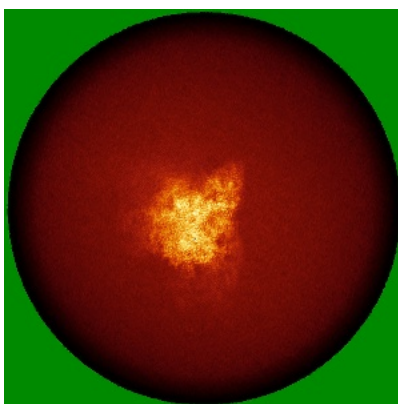


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

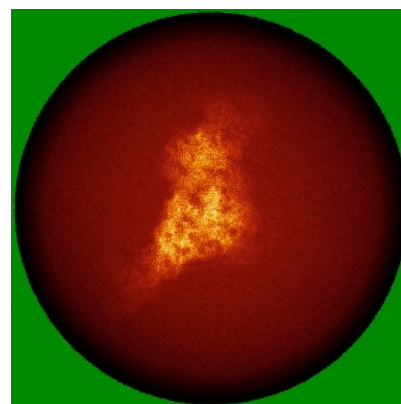
### 6.4.1 Primary map



X

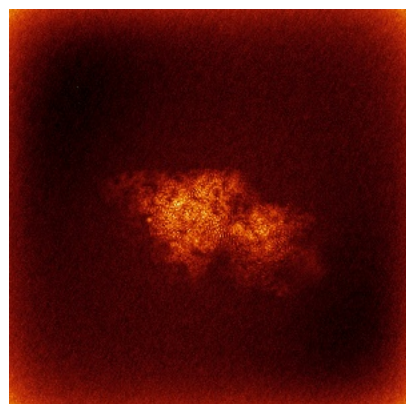


Y

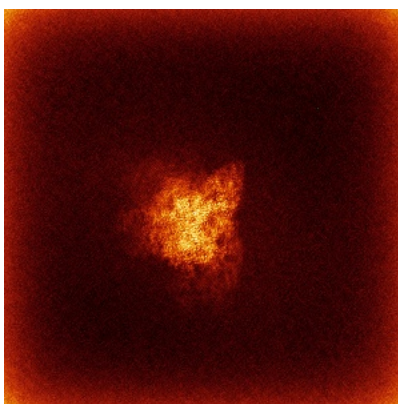


Z

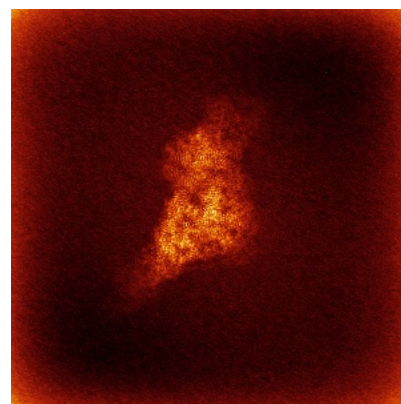
### 6.4.2 Raw map



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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0377. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

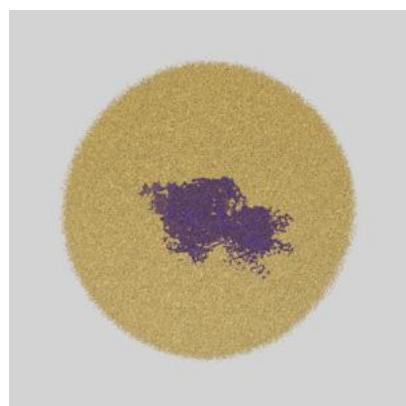
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

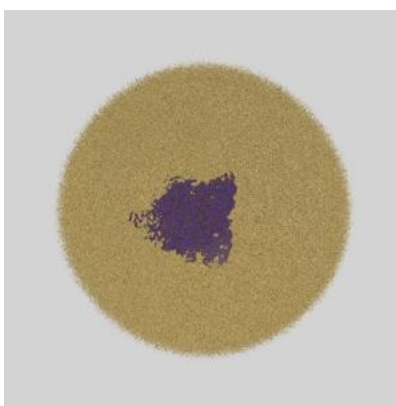
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

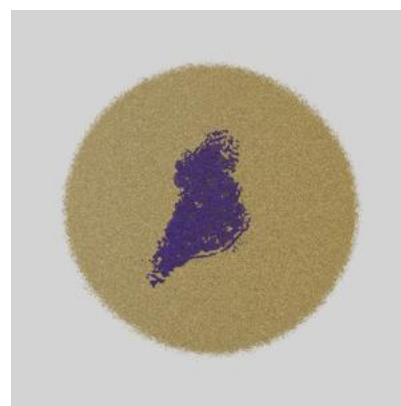
### 6.6.1 emd\_50014\_msk\_1.map [i](#)



X



Y

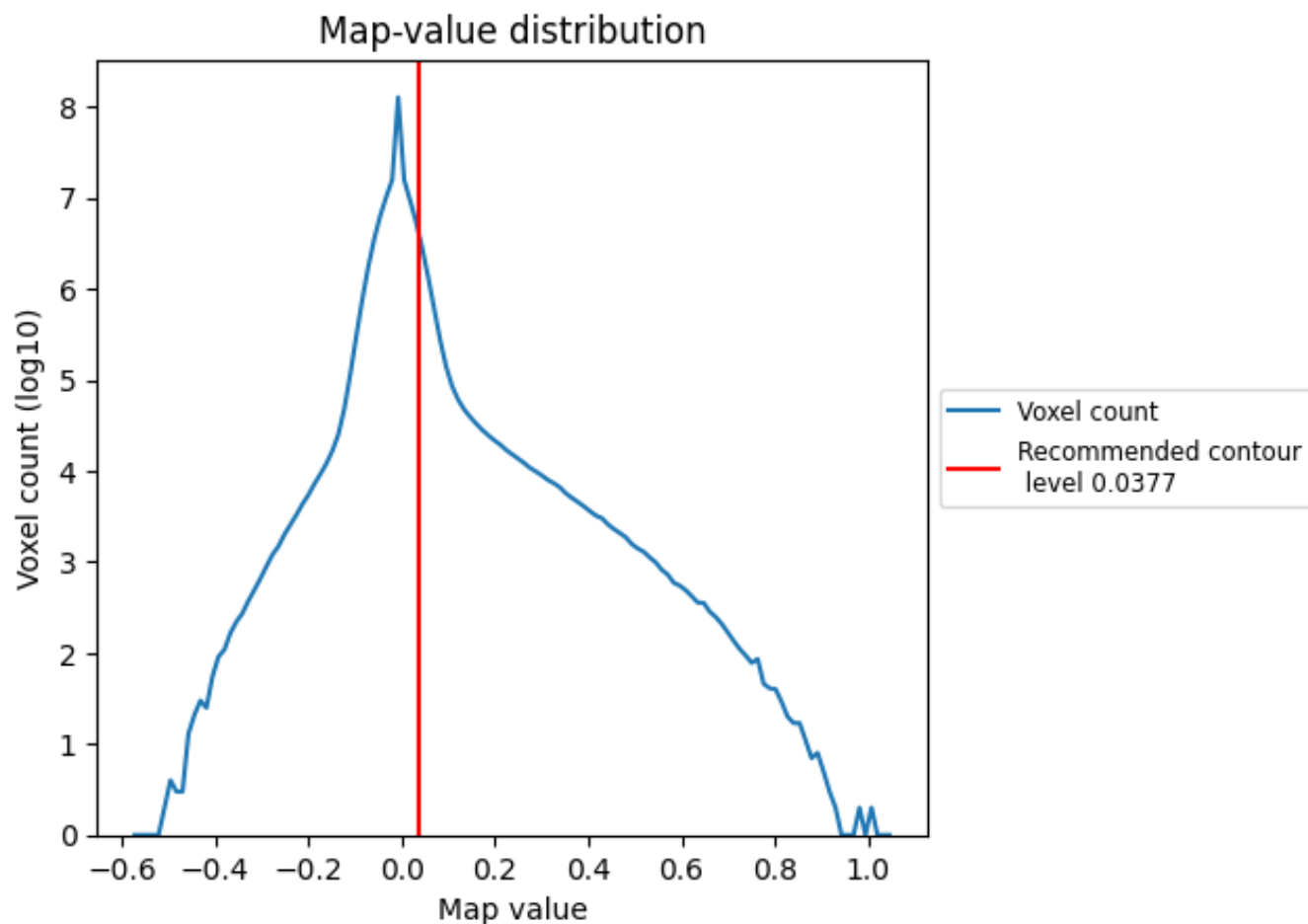


Z

## 7 Map analysis [i](#)

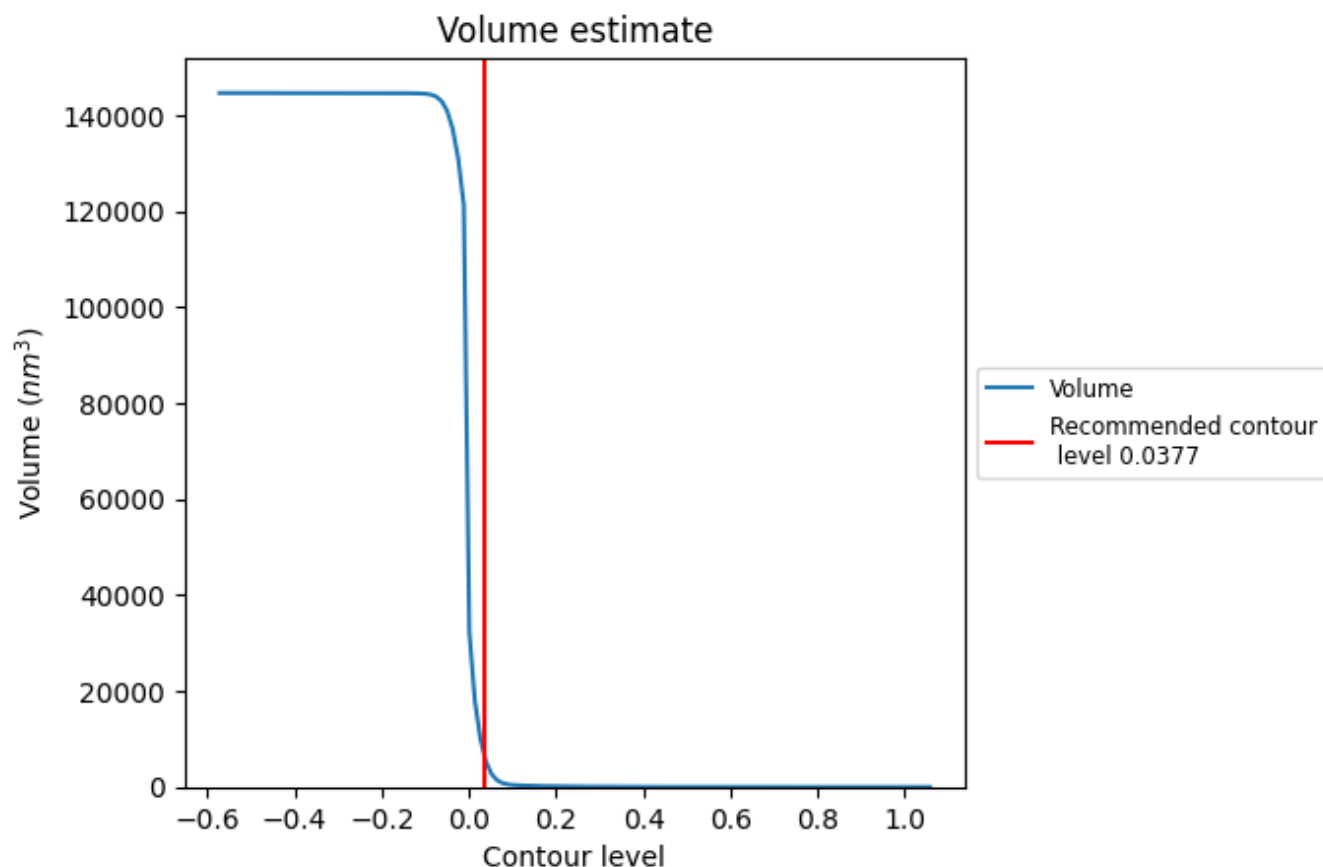
This section contains the results of statistical analysis of the map.

### 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.

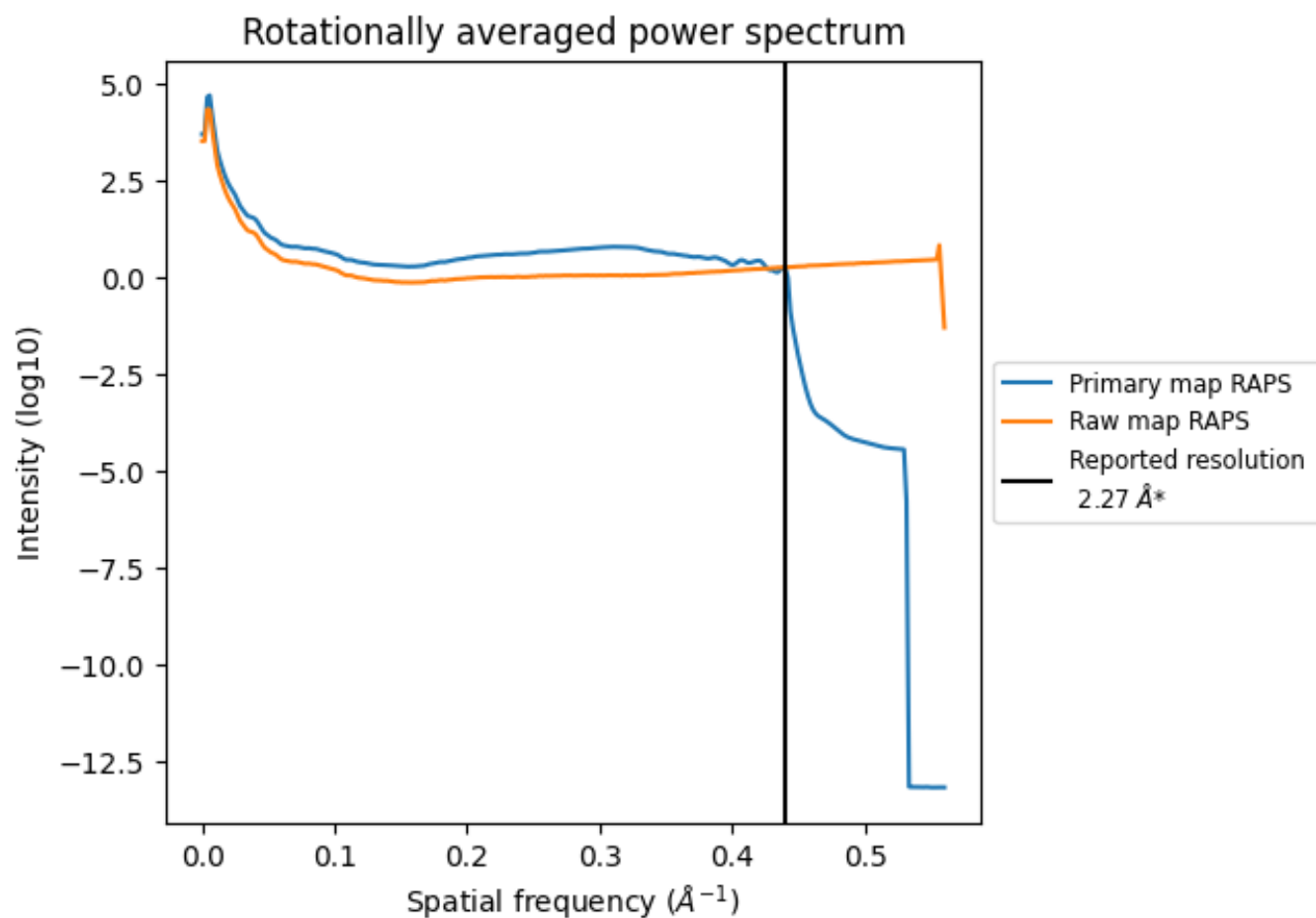
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5856 nm<sup>3</sup>; this corresponds to an approximate mass of 5290 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 ⓘ

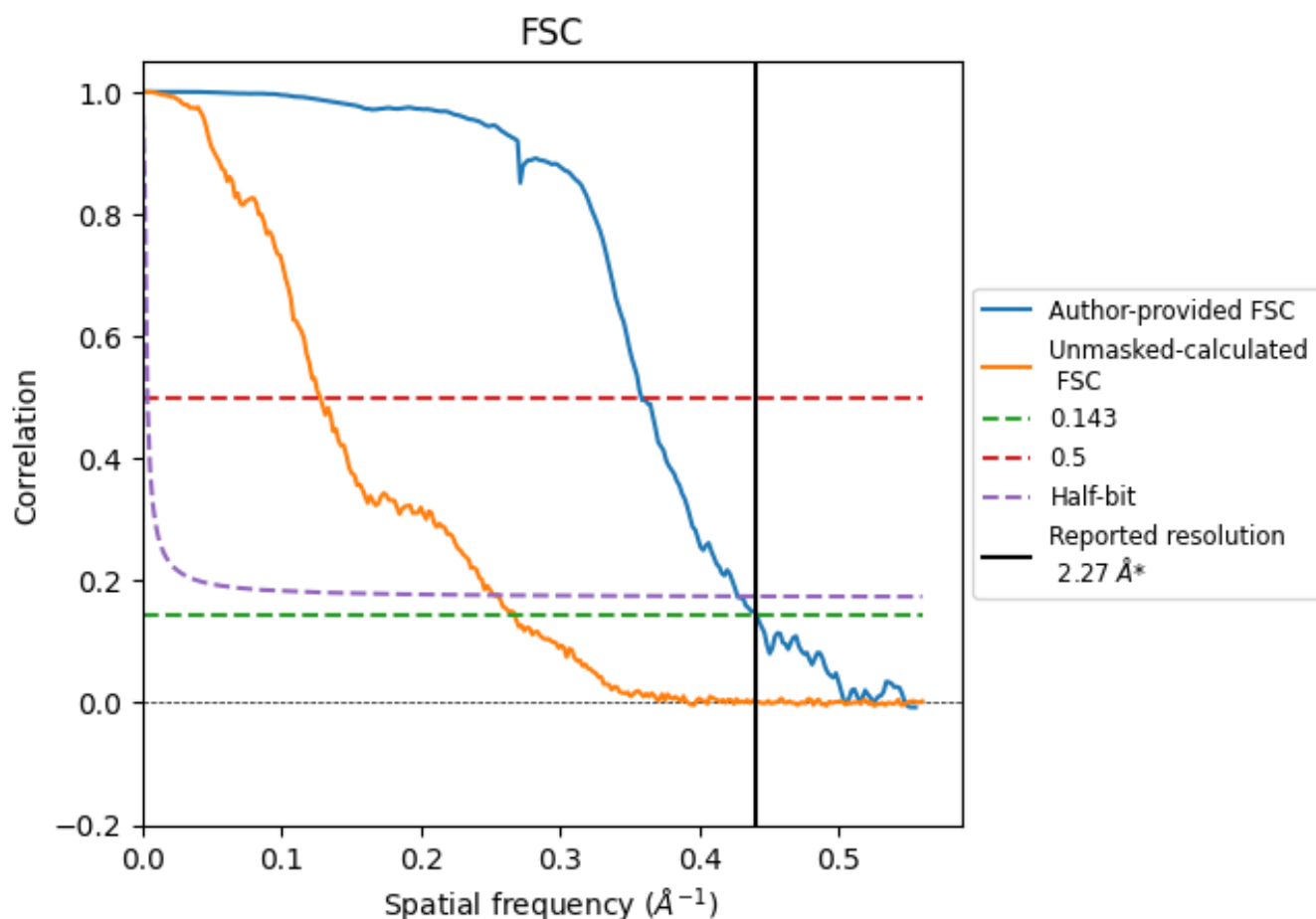


\*Reported resolution corresponds to spatial frequency of 0.441  $\text{\AA}^{-1}$

## 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 0.441  $\text{\AA}^{-1}$

## 8.2 Resolution estimates

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.27	-	-
Author-provided FSC curve	2.27	2.79	2.34
Unmasked-calculated*	3.74	7.82	3.95

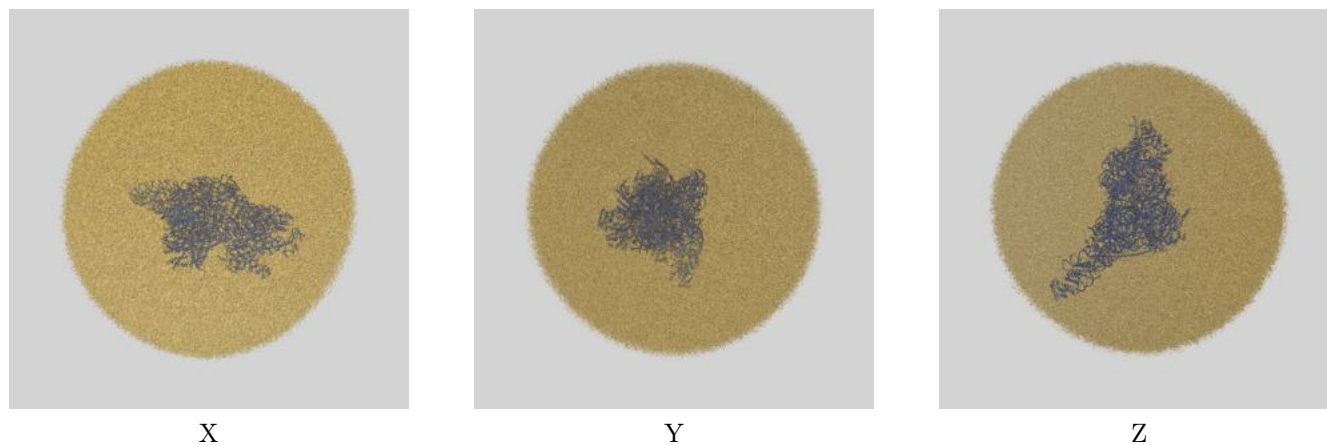
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.74 differs from the reported value 2.27 by more than 10 %



## 9 Map-model fit [i](#)

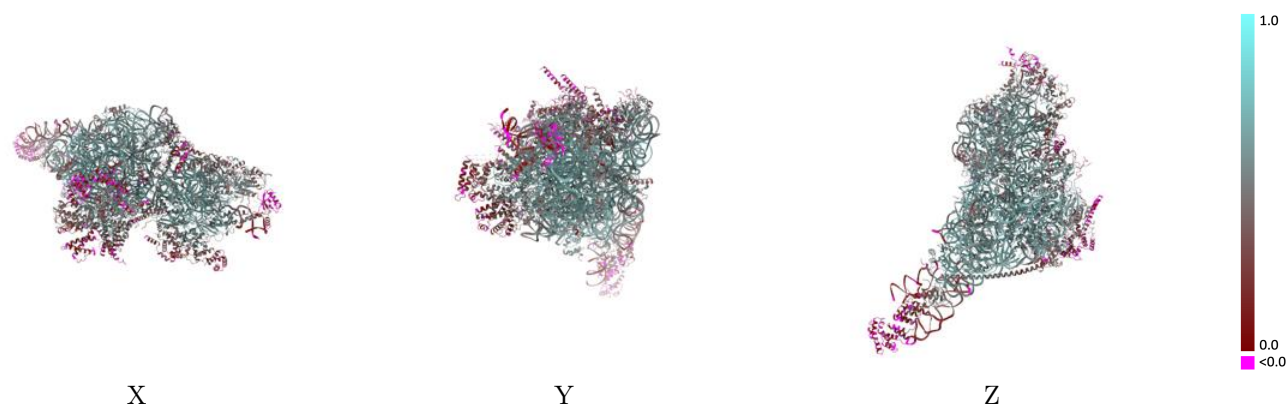
This section contains information regarding the fit between EMDB map EMD-50014 and PDB model 9EVT. Per-residue inclusion information can be found in section 3 on page 14.

### 9.1 Map-model overlay [i](#)



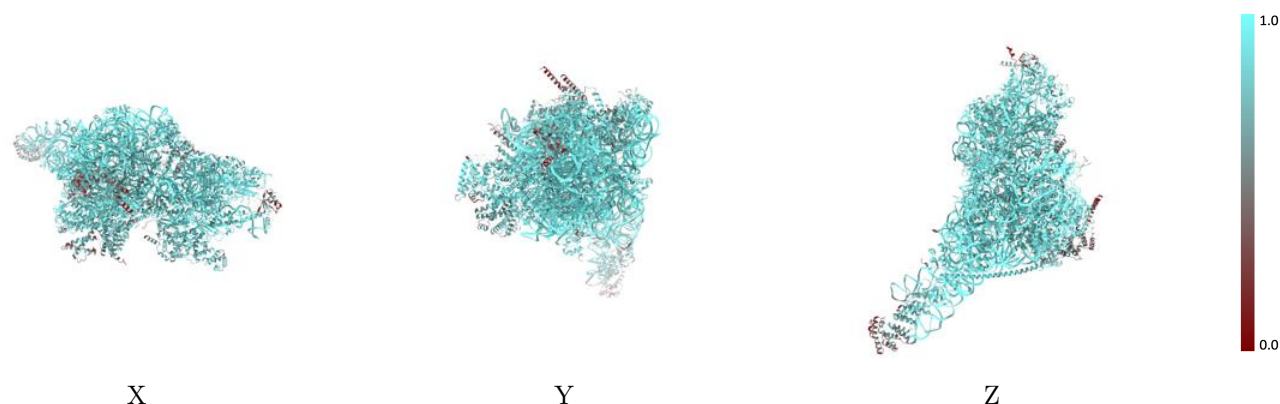
The images above show the 3D surface view of the map at the recommended contour level 0.0377 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



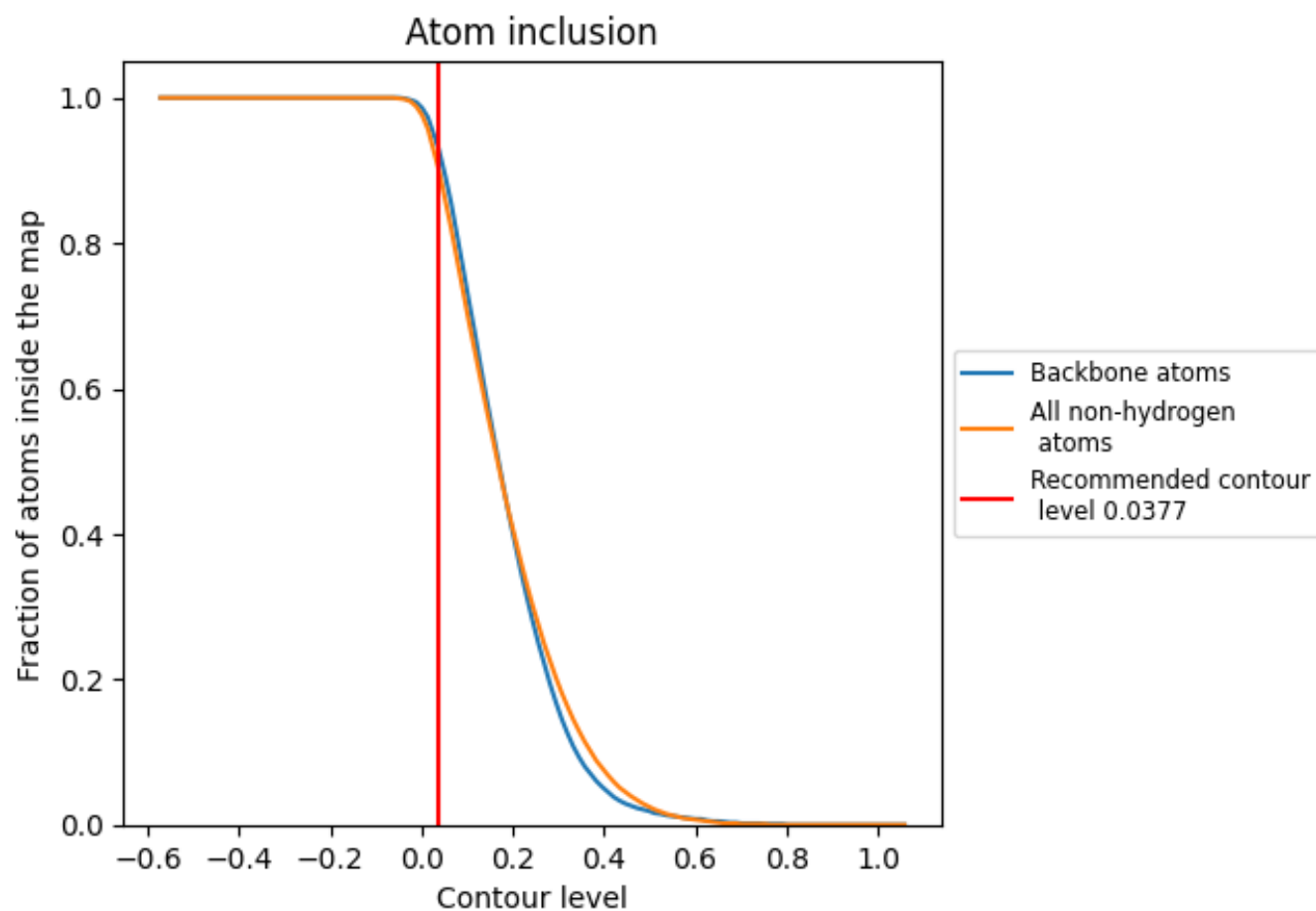
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0377).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 90% 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 (0.0377) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9010	 0.5020
2	 0.9740	 0.5800
7	 0.9100	 0.5250
A	 0.9270	 0.5410
B	 0.8560	 0.4390
C	 0.9460	 0.5680
D	 0.8790	 0.4990
E	 0.9420	 0.5380
F	 0.8380	 0.3910
G	 0.9690	 0.6320
H	 0.8250	 0.4610
I	 0.9630	 0.6190
J	 0.8640	 0.4510
K	 0.9590	 0.6220
L	 0.9010	 0.4900
M	 0.9680	 0.6220
N	 0.9220	 0.5590
O	 0.9820	 0.6530
P	 0.9430	 0.5960
Q	 0.8900	 0.5110
R	 0.6400	 0.2540
S	 0.8690	 0.4610
T	 0.9770	 0.6230
U	 0.6340	 0.2520
V	 0.8850	 0.4630
W	 0.8980	 0.4600
X	 0.8460	 0.4240
Y	 0.9150	 0.5370
Z	 0.9210	 0.4870
a	 0.8600	 0.4050
b	 0.5850	 0.1760
c	 0.8300	 0.4810
d	 0.9270	 0.5540
e	 0.9270	 0.5540
f	 0.8440	 0.3950



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Chain	Atom inclusion	Q-score
h	 0.6240	 0.1420
i	 0.5840	 0.1720
k	 0.8490	 0.3750