



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 07:09 AM UTC

PDB ID : 7WTZ / pdb_00007wtz
EMDB ID : EMD-32806
Title : Cryo-EM structure of a human pre-40S ribosomal subunit - State RRP12-B2
Authors : Cheng, J.; Lau, B.; Thoms, M.; Ameismeier, M.; Berninghausen, O.; Hurt, E.; Beckmann, R.
Deposited on : 2022-02-05
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

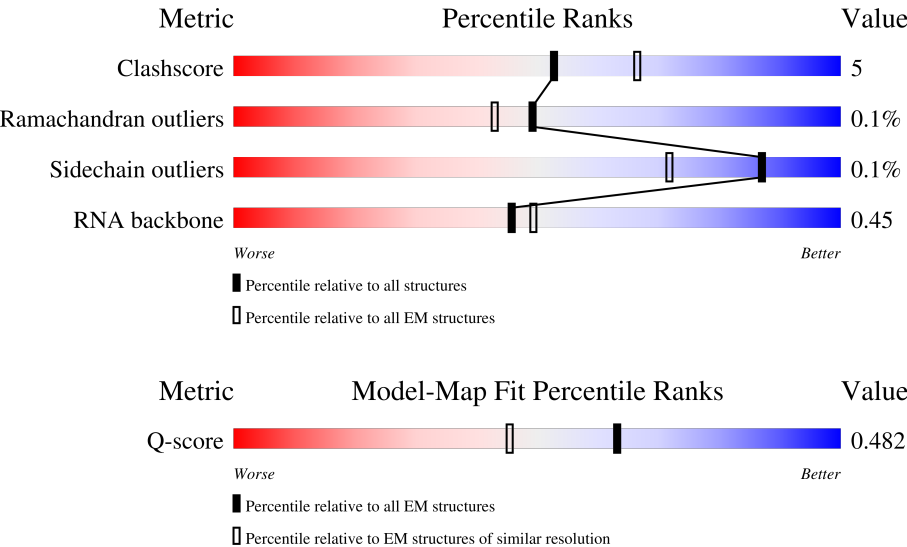
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.00 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	14081 (2.50 - 3.50)

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

Mol	Chain	Length	Quality of chain
1	2	1873	
2	F	204	
3	M	132	

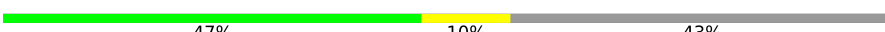
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Mol	Chain	Length	Quality of chain
4	P	145	
5	Q	146	
6	R	135	
7	S	152	
8	T	145	
9	Z	125	
10	c	69	
11	f	156	
12	A	295	
13	B	264	
14	C	293	
15	E	263	
16	G	249	
17	H	194	
18	I	208	
19	J	194	
20	L	158	
21	N	151	
22	O	151	
23	V	83	
24	W	130	
25	X	143	
26	Y	133	
27	b	84	
28	e	59	

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Mol	Chain	Length	Quality of chain
29	x	252	
30	y	412	
31	u	804	
32	w	437	
33	t	475	
34	K	1297	

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 85113 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 RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1624	Total	C	N	O	P	0	0
			34680	15479	6228	11350	1623		

- Molecule 2 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	189	Total	C	N	O	S	0	0
			1495	934	284	270	7		

- Molecule 3 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	123	Total	C	N	O	S	0	0
			953	598	169	177	9		

- Molecule 4 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	120	Total	C	N	O	S	0	0
			984	625	184	168	7		

- Molecule 5 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Q	122	Total	C	N	O	S	0	0
			969	616	180	170	3		

- Molecule 6 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	R	122	Total	C	N	O	S	0	0
			990	621	184	182	3		

- Molecule 7 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	S	130	Total	C	N	O	S	0	0
			1083	686	214	182	1		

- Molecule 8 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	T	144	Total	C	N	O	S	0	0
			1122	703	217	199	3		

- Molecule 9 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Z	72	Total	C	N	O	S	0	0
			574	368	104	101	1		

- Molecule 10 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	c	61	Total	C	N	O	S	0	0
			471	288	95	86	2		

- Molecule 11 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	f	73	Total	C	N	O	S	0	0
			596	375	115	99	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A	216	Total	C	N	O	S	0	0
			1705	1083	299	315	8		

- Molecule 13 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	B	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 14 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	C	218	Total	C	N	O	S	0	0
			1690	1094	289	297	10		

- Molecule 15 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	E	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 16 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	G	230	Total	C	N	O	S	0	0
			1862	1164	371	320	7		

- Molecule 17 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	H	186	Total	C	N	O	S	0	0
			1501	957	276	267	1		

- Molecule 18 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	I	205	Total	C	N	O	S	0	0
			1682	1056	331	290	5		

- Molecule 19 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	J	180	Total	C	N	O	S	0	0
			1499	955	300	242	2		

- Molecule 20 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	151	Total	C	N	O	S	0	0
			1229	782	230	211	6		

- Molecule 21 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	N	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 22 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	O	135	Total	C	N	O	S	0	0
			1009	618	198	187	6		

- Molecule 23 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	82	Total	C	N	O	S	0	0
			625	384	116	120	5		

- Molecule 24 is a protein called 40S ribosomal protein S15a.

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

- Molecule 25 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 26 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	124	Total	C	N	O	S	0	0
			1014	641	198	170	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	82	Total	C	N	O	S	0	0
			640	402	118	113	7		

- Molecule 28 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	55	Total	C	N	O	S	0	0
			438	271	95	71	1		

- Molecule 29 is a protein called RNA-binding protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	x	178	Total	C	N	O	S	0	0
			1391	891	252	244	4		

- Molecule 30 is a protein called RNA-binding protein NOB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	y	325	Total	C	N	O	S	0	0
			2568	1622	473	463	10		

- Molecule 31 is a protein called Pre-rRNA-processing protein TSR1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	u	629	Total	C	N	O	S	0	0
			5062	3249	902	887	24		

- Molecule 32 is a protein called Bystin.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	w	249	Total	C	N	O	S	0	0
			2027	1322	354	342	9		

- Molecule 33 is a protein called Protein LTV1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	t	127	Total	C	N	O	S	0	0
			1066	661	204	199	2		

- Molecule 34 is a protein called RRP12-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	K	909	Total	C	N	O	S	0	0
			7047	4520	1216	1266	45		

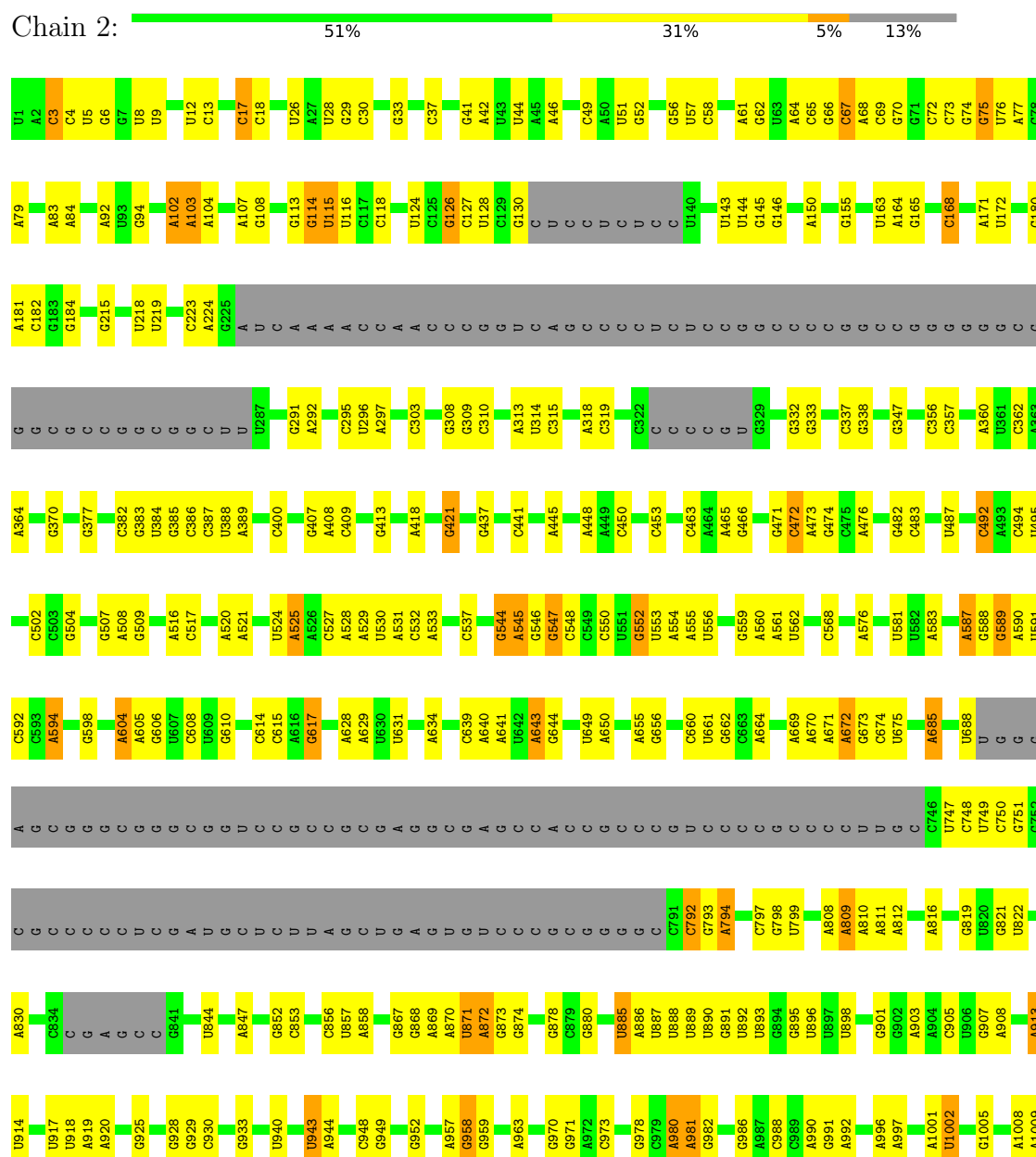
- Molecule 35 is ZINC ION (CCD ID: ZN) (formula: Zn).

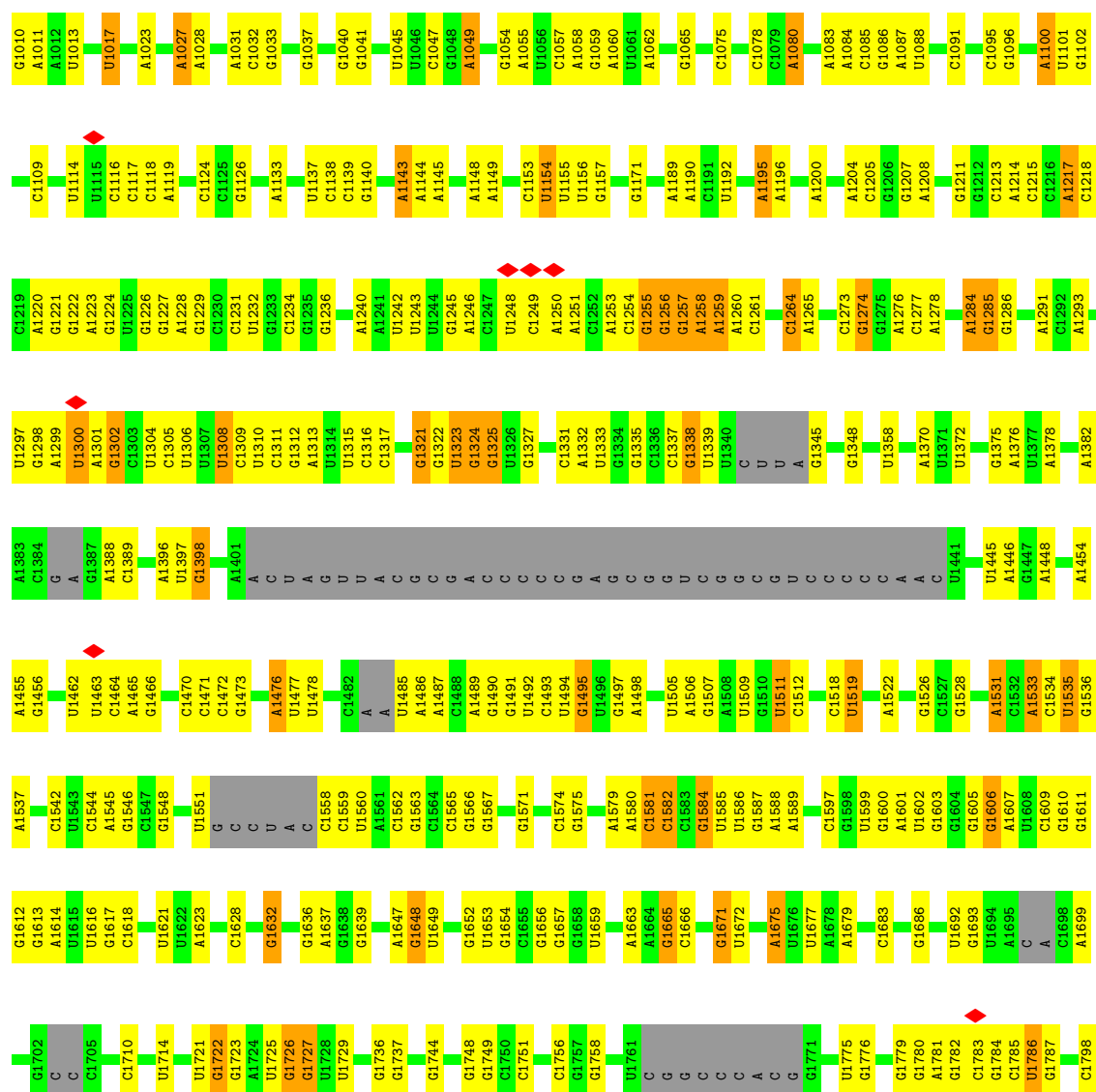
Mol	Chain	Residues	Atoms		AltConf
35	f	1	Total 1	Zn 1	0
35	y	1	Total 1	Zn 1	0

3 Residue-property plots [i](#)

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

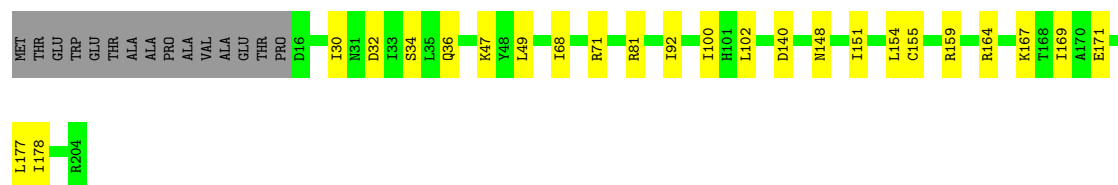
• Molecule 1: 18S rRNA





• Molecule 2: 40S ribosomal protein S5

Chain F: 81% 12% 7%

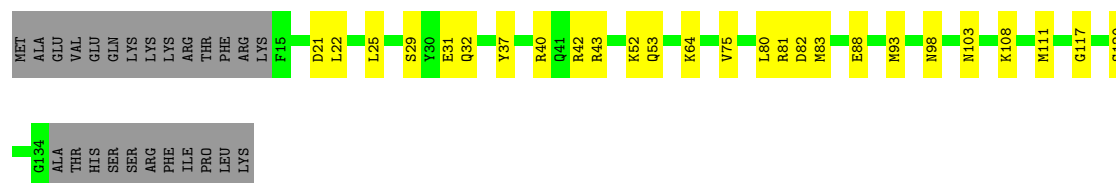


• Molecule 3: 40S ribosomal protein S12

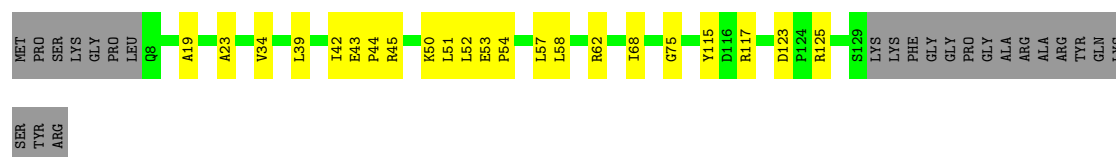
Chain M: 83% 11% 7%



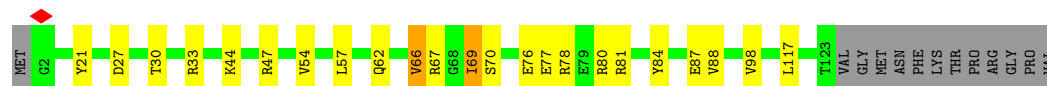
- Molecule 4: 40S ribosomal protein S15



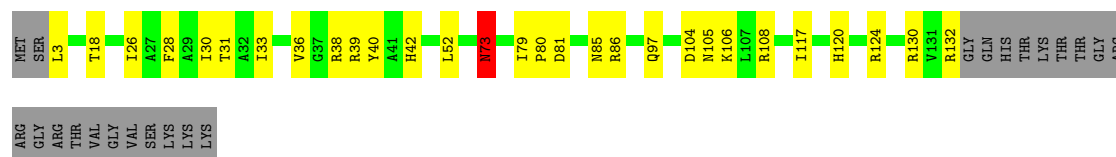
- Molecule 5: 40S ribosomal protein S16



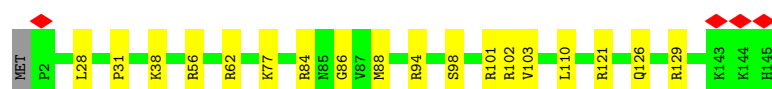
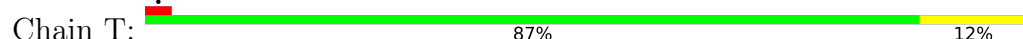
- Molecule 6: 40S ribosomal protein S17



- Molecule 7: 40S ribosomal protein S18

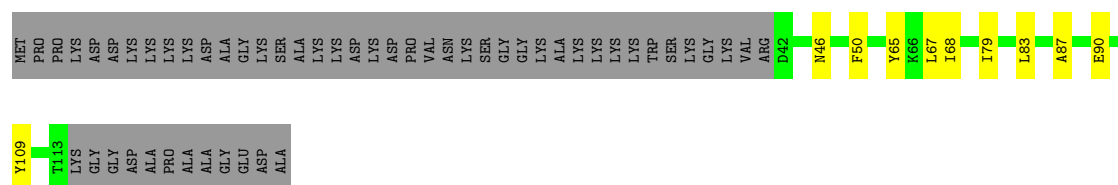


- Molecule 8: 40S ribosomal protein S19



- Molecule 9: 40S ribosomal protein S25

Chain Z:  50% 8% 42%



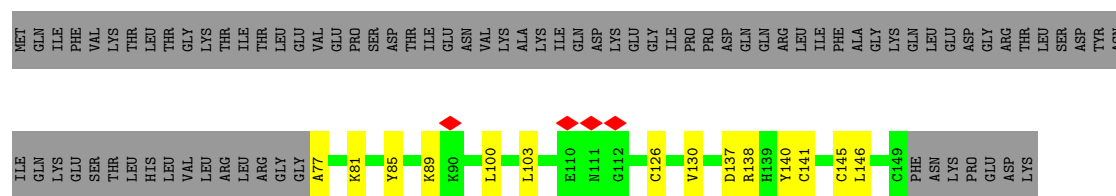
- Molecule 10: 40S ribosomal protein S28

Chain c:  77% 12% 12%



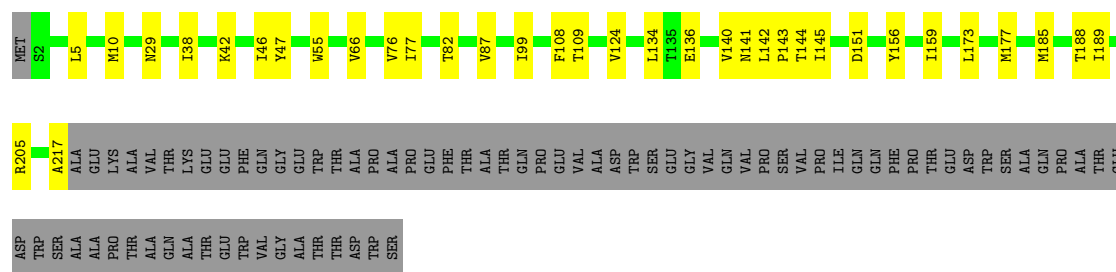
- Molecule 11: Ubiquitin-40S ribosomal protein S27a

Chain f:  38% 9% 53%



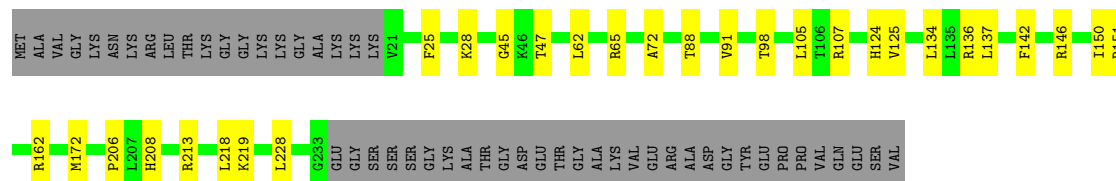
- Molecule 12: 40S ribosomal protein SA

Chain A:  61% 12% 27%



- Molecule 13: 40S ribosomal protein S3a

Chain B:  70% 11% 19%



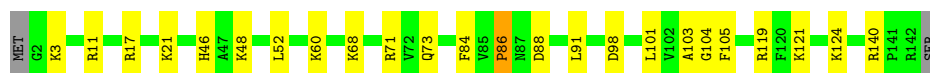
- Molecule 14: 40S ribosomal protein S2

T276	HIS	R65
THR	ARG	L66
VAL	ARG	I81
SER	VAL	L107
VAL	GLN	K108
THR	ARG	G131
ARG	THR	G136
GLN	ALA	H136
ALA	PRO	V137
VAL	ALA	G
VAL	VAL	V165
ALA	ALA	R166
THR	THR	M172
THR		K183
		R187
		S190
		V191
		L192
		G
		L195
		I196
		V209
		M216
		A217
		D221
		C222
		V223
		G
		R227
		T230
		L233
		D242
		A243
		I244
		S245
		K246
		T247
		Y248
		S249
		V250
		L251
		G
		D271
		H272
		L273

- | MIT |
|------|
| A2 |
| R11 |
| D21 |
| A28 |
| P31 |
| L38 |
| I45 |
| R49 |
| V61 |
| I80 |
| G107 |
| V126 |
| A127 |
| K128 |
| V131 |
| G132 |
| L139 |
| V140 |
| T141 |
| P152 |
| I162 |
| I169 |
| C181 |
| L189 |
| I195 |
| D206 |
| A219 |
| L222 |
| A263 |

- | | | | | | | | | | | | | | | | | | | |
|----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| M1 | K2 | F7 | G11 | L15 | D19 | K23 | L24 | L41 | G42 | E43 | Y48 | V49 | V50 | N56 | D57 | X58 | Q59 | R72 | S78 | R85 | P86 | R87 | R92 | V102 | L106 | S107 | V108 | I113 | V114 | K115 | K116 | K119 | D120 | I121 | L124 | R132 | L133 | G134 | P135 | V136 |
| | I141 | L144 | Q155 | L162 | M163 | K164 | K168 | K172 | K175 | L176 | Q177 | R178 | R198 | K201 | A214 | K215 | R216 | E219 | E222 | I228 | A229 | K230 | ARG | ARG | ARG | ARG | LEU | LEU | ARG | ALA | SER | THR | SER | LYS | SER | GLU | SER | SER | GLN | LYS |

-
- Amino acid residues
- Disordered regions
- MET
- G2
- I3
- S4
- R5
- D6
- K19
- P20
- G30
- R42
- V48
- K54
- A57
- L58
- R59
- L60
- D61
- S69
- N84
- N88
- E89
- L90
- Y91
- R92
- I101
- V102
- L103
- I104
- D105
- S106
- L119
- K125
- A126
- I127
- K128
- K139
- K140
- R141
- S142
- I145
- K153
- K154
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- C174
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- R184
- L190
- E191
- R205
- K206
- GLY
- LYS



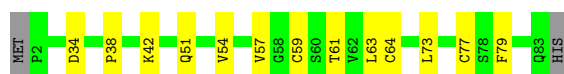
- Molecule 26: 40S ribosomal protein S24

Chain Y: 80% 13% 7%



- Molecule 27: 40S ribosomal protein S27

Chain b: 82% 15% .



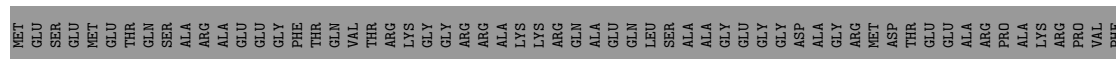
- Molecule 28: 40S ribosomal protein S30

Chain e: 85% 8% 7%



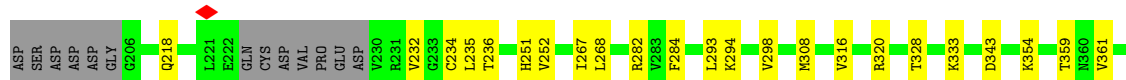
- Molecule 29: RNA-binding protein PNO1

Chain x: 62% 8% 29%

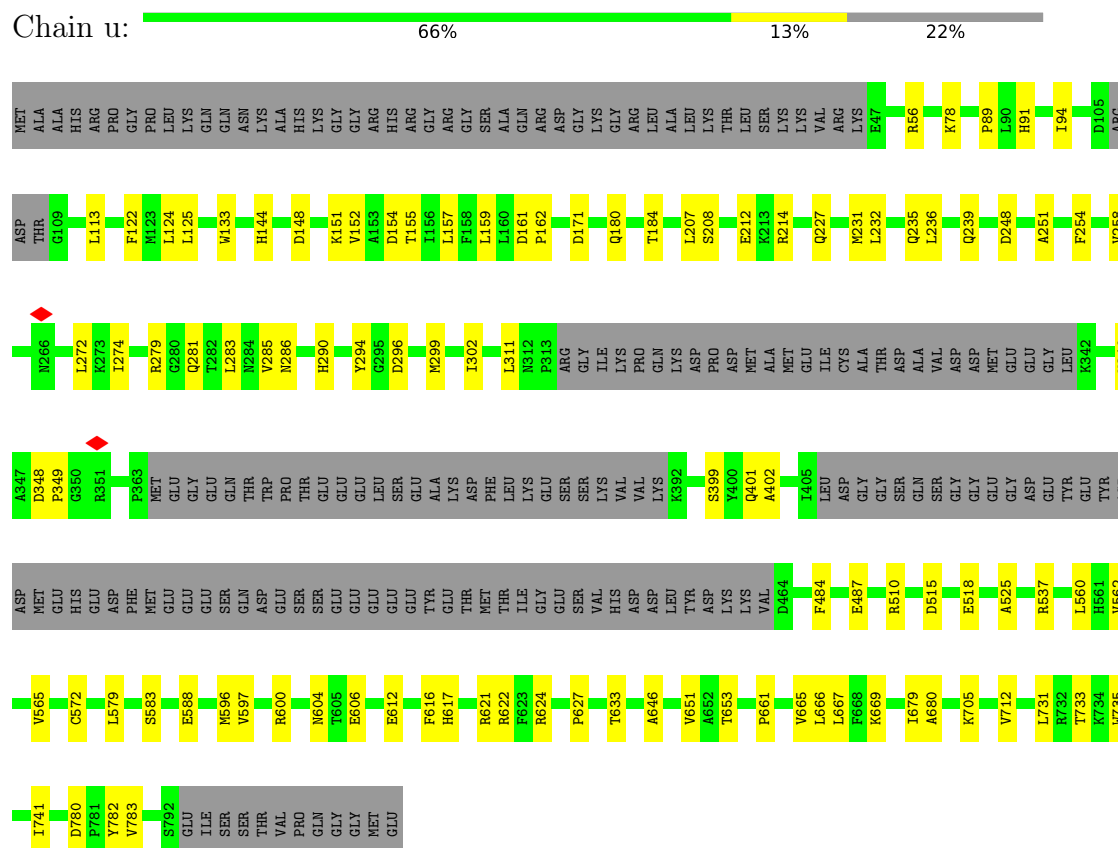


- Molecule 30: RNA-binding protein NOB1

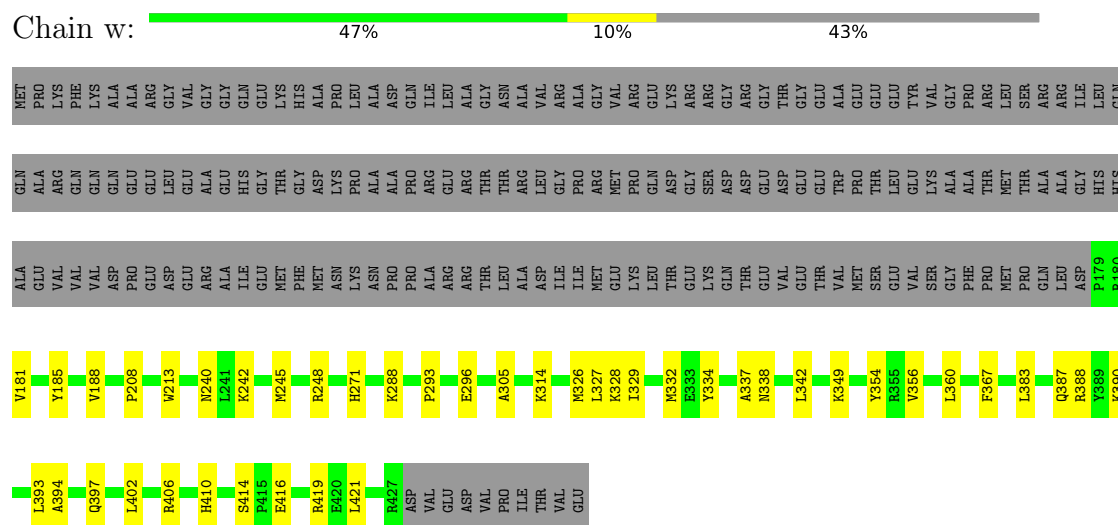
Chain y: 66% 13% 21%



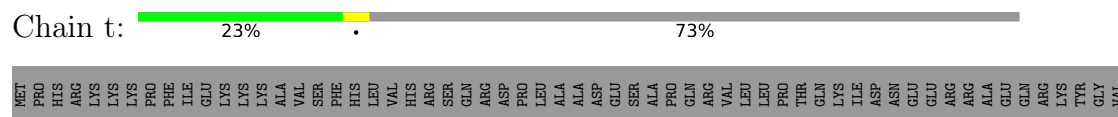
- Molecule 31: Pre-rRNA-processing protein TSR1 homolog

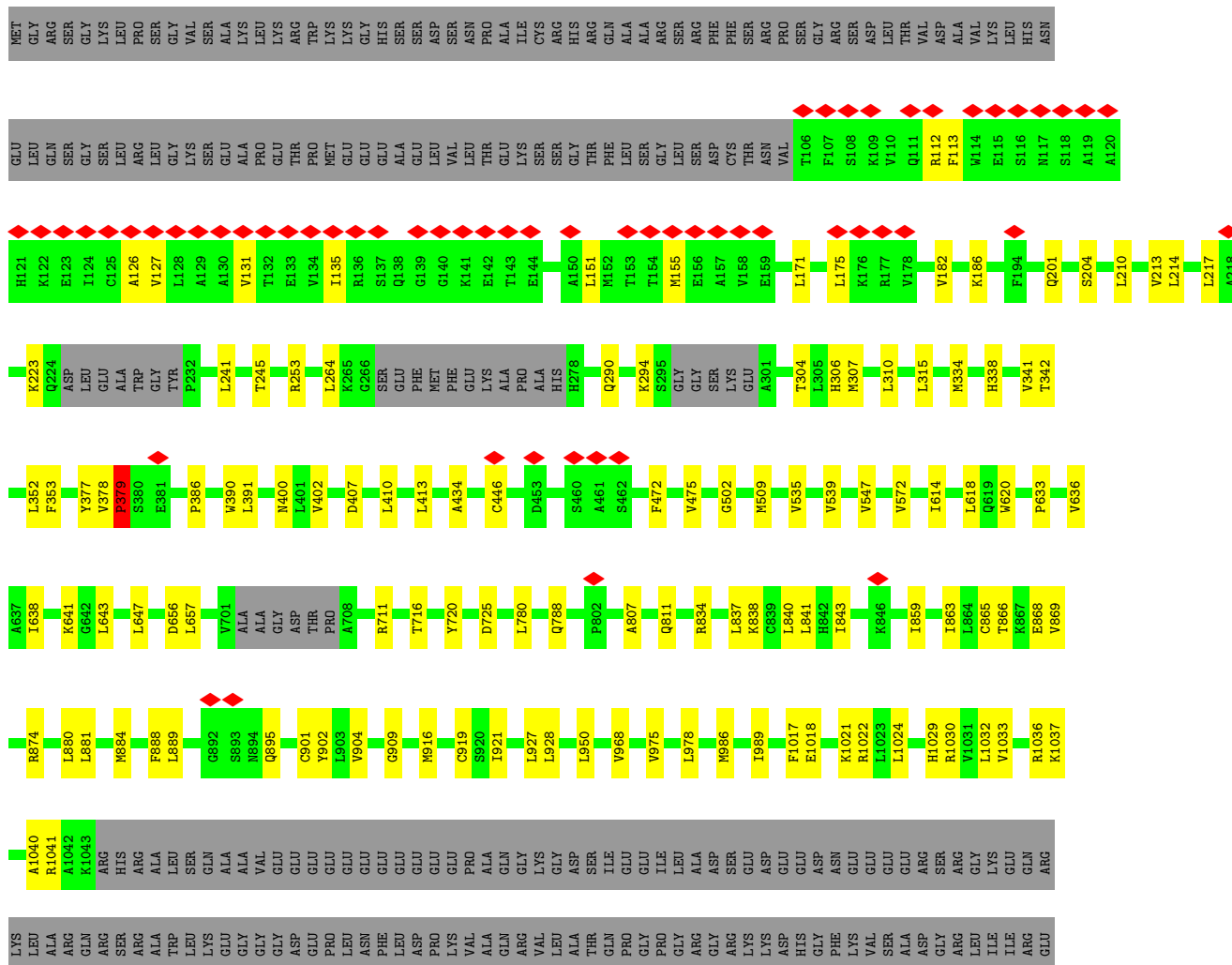


- Molecule 32: Bystin



- Molecule 33: Protein LTV1 homolog





[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	48362	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Relion	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.516	Depositor
Minimum map value	-0.257	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	381.24, 381.24, 381.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
ZN

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	2	0.20	0/38775	0.37	0/60417
2	F	0.17	0/1516	0.50	0/2037
3	M	0.16	0/963	0.47	0/1291
4	P	0.22	0/1003	0.56	0/1341
5	Q	0.18	0/982	0.50	0/1318
6	R	0.44	0/1002	0.73	0/1345
7	S	0.19	0/1100	0.55	1/1475 (0.1%)
8	T	0.19	0/1142	0.48	0/1530
9	Z	0.19	0/580	0.57	0/780
10	c	0.17	0/473	0.50	0/633
11	f	0.17	0/607	0.50	0/802
12	A	0.25	0/1742	0.54	0/2367
13	B	0.18	0/1756	0.49	1/2350 (0.0%)
14	C	0.24	0/1726	0.53	0/2332
15	E	0.23	0/2118	0.55	0/2849
16	G	0.21	0/1885	0.55	0/2510
17	H	0.20	0/1524	0.52	0/2042
18	I	0.23	0/1711	0.53	0/2282
19	J	0.22	0/1524	0.49	0/2035
20	L	0.21	0/1250	0.49	0/1673
21	N	0.19	0/1226	0.38	0/1649
22	O	0.25	0/1022	0.59	0/1372
23	V	0.18	0/631	0.46	0/844
24	W	0.24	0/1051	0.61	0/1406
25	X	0.24	0/1116	0.62	4/1490 (0.3%)
26	Y	0.20	0/1031	0.49	0/1370
27	b	0.21	0/653	0.58	0/876
28	e	0.18	0/443	0.53	0/582
29	x	0.23	0/1413	0.53	0/1906
30	y	0.23	0/2618	0.60	1/3536 (0.0%)
31	u	0.22	0/5187	0.52	0/7011
32	w	0.20	0/2074	0.50	0/2806

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	t	0.23	0/1075	0.62	0/1424
34	K	0.22	0/7182	0.57	1/9732 (0.0%)
All	All	0.21	0/90101	0.47	8/129413 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	y	60	PRO	CA-N-CD	-9.35	98.91	112.00
13	B	45	GLY	N-CA-C	6.30	118.64	110.45
25	X	104	GLY	CA-C-N	-5.51	113.07	122.11
25	X	104	GLY	C-N-CA	-5.51	113.07	122.11
7	S	73	ASN	CB-CA-C	5.31	117.24	110.34
25	X	60	LYS	CA-C-N	5.19	129.77	121.62
25	X	60	LYS	C-N-CA	5.19	129.77	121.62
34	K	379	PRO	N-CA-CB	-5.10	97.89	103.25

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	34680	0	17507	286	0
2	F	1495	0	1549	15	0
3	M	953	0	990	9	0
4	P	984	0	1028	20	0
5	Q	969	0	1030	16	0
6	R	990	0	1037	25	0
7	S	1083	0	1140	21	0
8	T	1122	0	1153	15	0
9	Z	574	0	627	7	0
10	c	471	0	499	7	0
11	f	596	0	627	10	0
12	A	1705	0	1706	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	B	1729	0	1803	17	0
14	C	1690	0	1777	23	0
15	E	2076	0	2177	18	0
16	G	1862	0	2018	40	0
17	H	1501	0	1593	19	0
18	I	1682	0	1769	22	0
19	J	1499	0	1618	25	0
20	L	1229	0	1302	9	0
21	N	1202	0	1289	13	0
22	O	1009	0	1034	17	0
23	V	625	0	628	7	0
24	W	1034	0	1080	15	0
25	X	1098	0	1167	14	0
26	Y	1014	0	1082	11	0
27	b	640	0	665	7	0
28	e	438	0	484	4	0
29	x	1391	0	1467	14	0
30	y	2568	0	2624	33	0
31	u	5062	0	5113	62	0
32	w	2027	0	2126	28	0
33	t	1066	0	1070	15	0
34	K	7047	0	7310	84	0
35	f	1	0	0	0	0
35	y	1	0	0	0	0
All	All	85113	0	70089	793	0

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

All (793) 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)
24:W:101:PHE:O	24:W:128:PHE:HA	1.39	1.21
1:2:533:A:H61	1:2:550:C:N4	1.52	1.07
1:2:1710:C:H42	1:2:1823:A:N6	1.52	1.05
1:2:533:A:N6	1:2:550:C:H42	1.54	1.04
1:2:1710:C:N4	1:2:1823:A:H61	1.59	0.98
22:O:42:VAL:O	22:O:55:ARG:HA	1.64	0.97
6:R:21:TYR:CE2	6:R:69:ILE:HG23	2.00	0.96
1:2:1710:C:H42	1:2:1823:A:H61	0.96	0.90
1:2:685:A:N6	1:2:917:U:H3	1.71	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:8:U:N3	1:2:1196:A:N6	2.21	0.88
1:2:1398:G:H1	1:2:1448:A:H2	1.23	0.87
1:2:685:A:N6	1:2:917:U:N3	2.27	0.82
1:2:8:U:H3	1:2:1196:A:N6	1.78	0.82
6:R:21:TYR:OH	6:R:69:ILE:HD12	1.81	0.80
14:C:183:LYS:HA	14:C:195:LEU:O	1.83	0.78
1:2:8:U:C4	1:2:1196:A:N6	2.54	0.76
1:2:1245:G:C6	1:2:1255:G:N2	2.53	0.76
1:2:1710:C:N3	1:2:1823:A:N1	2.37	0.72
1:2:1236:G:H21	1:2:1522:A:H62	1.38	0.72
1:2:1259:A:N6	1:2:1519:U:OP1	2.23	0.71
1:2:1333:U:O2	1:2:1495:G:N2	2.25	0.69
1:2:1091:C:HO2'	24:W:2:VAL:N	1.90	0.69
4:P:108:LYS:H	4:P:111:MET:HE2	1.56	0.69
6:R:21:TYR:CZ	6:R:69:ILE:HD12	2.28	0.69
1:2:928:G:H1	1:2:1013:U:H3	1.40	0.68
1:2:952:G:H21	22:O:52:THR:HG21	1.58	0.68
31:u:600:ARG:NH2	31:u:606:GLU:O	2.27	0.68
4:P:111:MET:HB3	7:S:117:ILE:HG12	1.76	0.67
1:2:1137:U:H5''	30:y:328:THR:HG23	1.75	0.67
30:y:16:ARG:HH11	30:y:218:GLN:HE21	1.41	0.67
1:2:957:A:H3'	1:2:958:G:H21	1.59	0.67
2:F:92:ILE:HD13	2:F:169:ILE:HD11	1.77	0.66
17:H:51:ILE:HD11	17:H:176:VAL:HG12	1.76	0.66
5:Q:23:ALA:HB1	5:Q:68:ILE:HD11	1.77	0.66
7:S:105:ASN:OD1	7:S:108:ARG:NH2	2.29	0.66
11:f:141:CYS:HB3	11:f:146:LEU:H	1.60	0.65
4:P:75:VAL:HA	4:P:93:MET:O	1.95	0.65
25:X:71:ARG:HH22	33:t:471:GLU:H	1.45	0.65
1:2:533:A:N1	1:2:550:C:N3	2.44	0.65
1:2:65:C:N4	16:G:134:GLY:O	2.30	0.65
17:H:69:LEU:HD22	17:H:96:ALA:HB2	1.79	0.65
5:Q:53:GLU:O	5:Q:57:LEU:HB2	1.97	0.64
18:I:101:ILE:HD12	18:I:190:LEU:HD11	1.78	0.64
34:K:863:ILE:HG22	34:K:919:CYS:HB3	1.77	0.64
21:N:55:ARG:NH2	27:b:51:GLN:OE1	2.29	0.64
31:u:125:LEU:HD11	31:u:311:LEU:HA	1.77	0.64
32:w:416:GLU:HG2	32:w:419:ARG:HH12	1.63	0.64
16:G:7:PHE:HD1	16:G:113:ILE:HD11	1.63	0.64
25:X:98:ASP:OD2	25:X:140:ARG:NH2	2.31	0.64
6:R:21:TYR:HE2	6:R:69:ILE:CG2	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:925:G:H1	1:2:1017:U:H3	1.46	0.64
6:R:21:TYR:HE2	6:R:69:ILE:HG23	1.56	0.64
32:w:394:ALA:H	32:w:397:GLN:HE21	1.46	0.64
10:c:32:VAL:O	10:c:41:SER:HA	1.98	0.63
1:2:561:A:HO2'	19:J:134:HIS:HE2	1.42	0.63
31:u:733:THR:HG22	31:u:735:TRP:H	1.63	0.63
4:P:52:LYS:HG3	4:P:80:LEU:HD11	1.79	0.63
1:2:1156:U:OP1	24:W:71:LYS:NZ	2.32	0.63
31:u:154:ASP:OD2	31:u:279:ARG:NH2	2.32	0.63
1:2:64:A:H2	1:2:83:A:H62	1.47	0.62
1:2:67:C:H41	16:G:163:ASN:HA	1.63	0.62
1:2:925:G:OP1	21:N:121:ARG:NH1	2.33	0.62
1:2:940:U:H3	1:2:1002:U:H3	1.46	0.62
7:S:86:ARG:HH11	7:S:106:LYS:HE2	1.63	0.62
34:K:807:ALA:O	34:K:811:GLN:NE2	2.33	0.62
6:R:21:TYR:CE2	6:R:69:ILE:CG2	2.79	0.62
1:2:164:A:H3'	1:2:165:G:H21	1.65	0.62
1:2:492:C:N4	1:2:507:G:OP2	2.24	0.62
1:2:1599:U:OP2	9:Z:46:ASN:ND2	2.33	0.62
13:B:72:ALA:HB3	22:O:128:ARG:HH22	1.65	0.62
31:u:617:HIS:HB2	31:u:666:LEU:HB2	1.82	0.61
1:2:1264:C:N4	1:2:1518:C:N3	2.47	0.61
1:2:1398:G:N1	1:2:1448:A:C2	2.63	0.61
29:x:205:ALA:HB3	29:x:208:LYS:HB2	1.81	0.61
1:2:103:A:OP2	1:2:356:C:N4	2.29	0.61
6:R:66:VAL:HG21	34:K:614:ILE:HG23	1.82	0.61
34:K:334:MET:HE1	34:K:342:THR:HA	1.82	0.61
19:J:111:GLN:HE21	19:J:123:ILE:HG13	1.64	0.61
1:2:1045:U:OP2	33:t:420:LYS:NZ	2.34	0.61
12:A:38:ILE:HD11	12:A:47:TYR:HB3	1.83	0.61
12:A:156:TYR:HA	23:V:60:ARG:HG2	1.83	0.61
20:L:119:ASP:O	20:L:147:LYS:NZ	2.34	0.61
1:2:1276:A:H5'	32:w:314:LYS:HA	1.82	0.60
14:C:242:ASP:OD1	14:C:246:LYS:NZ	2.33	0.60
31:u:283:LEU:HD21	31:u:560:LEU:HD21	1.83	0.60
31:u:78:LYS:HG2	31:u:311:LEU:HD23	1.83	0.60
1:2:126:G:OP1	16:G:198:ARG:NH1	2.34	0.60
31:u:705:LYS:HB2	31:u:712:VAL:HB	1.83	0.60
22:O:106:LYS:HE3	22:O:136:PRO:HD2	1.84	0.60
34:K:837:LEU:HA	34:K:840:LEU:HD12	1.84	0.60
1:2:1486:A:C6	1:2:1487:A:N6	2.69	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:u:227:GLN:NE2	31:u:231:MET:SD	2.74	0.60
1:2:1839:U:OP2	29:x:236:LYS:NZ	2.35	0.60
32:w:185:TYR:HA	32:w:188:VAL:HG12	1.83	0.59
12:A:124:VAL:HG11	12:A:134:LEU:HD21	1.84	0.59
16:G:59:GLN:OE1	16:G:72:ARG:NH2	2.35	0.59
17:H:145:ARG:NH2	24:W:49:GLU:OE2	2.34	0.59
34:K:402:VAL:HG21	34:K:446:CYS:HB3	1.83	0.59
22:O:106:LYS:HD2	22:O:135:ILE:HG22	1.84	0.59
1:2:1311:C:H41	3:M:36:ARG:HH22	1.48	0.59
15:E:126:VAL:HA	15:E:141:THR:HA	1.85	0.59
26:Y:4:THR:OG1	26:Y:32:LYS:NZ	2.35	0.59
1:2:1613:G:OP1	4:P:42:ARG:NH1	2.31	0.58
1:2:532:C:H5'	32:w:406:ARG:HG3	1.85	0.58
6:R:66:VAL:HG11	34:K:618:LEU:HD21	1.85	0.58
1:2:1472:C:OP2	34:K:834:ARG:NH2	2.36	0.58
16:G:121:ILE:HG21	16:G:124:LEU:HD12	1.84	0.58
34:K:502:GLY:HA2	34:K:509:MET:HE1	1.85	0.58
1:2:1060:A:O2'	1:2:1062:A:N6	2.36	0.58
1:2:1486:A:N6	1:2:1487:A:N6	2.51	0.58
31:u:484:PHE:HB3	31:u:487:GLU:HG3	1.85	0.58
1:2:1192:U:OP2	25:X:119:ARG:NH2	2.29	0.58
10:c:13:ARG:HB3	10:c:33:GLU:HB3	1.86	0.58
1:2:1679:A:OP1	10:c:20:ARG:NH2	2.36	0.58
30:y:298:VAL:HG12	30:y:308:MET:HG2	1.84	0.58
17:H:60:ILE:HD11	17:H:92:VAL:HG22	1.86	0.58
31:u:235:GLN:NE2	31:u:239:GLN:OE1	2.29	0.58
34:K:217:LEU:HB3	34:K:241:LEU:HD21	1.85	0.58
13:B:125:VAL:HG22	13:B:172:MET:HE3	1.85	0.58
21:N:99:ARG:HE	21:N:115:LEU:HD21	1.69	0.58
1:2:928:G:H2'	1:2:929:G:C8	2.39	0.58
16:G:136:LYS:NZ	16:G:175:LYS:O	2.34	0.58
1:2:525:A:N7	1:2:589:G:O6	2.37	0.57
15:E:11:ARG:HA	15:E:28:ALA:HB2	1.86	0.57
17:H:158:LEU:HD11	17:H:187:PHE:HD2	1.69	0.57
1:2:1075:C:OP1	21:N:107:LYS:NZ	2.37	0.57
4:P:103:ASN:ND2	31:u:401:GLN:OE1	2.37	0.57
7:S:124:ARG:NH1	7:S:130:ARG:O	2.37	0.57
13:B:134:LEU:HB3	13:B:219:LYS:HB3	1.86	0.57
15:E:11:ARG:HH21	15:E:21:ASP:H	1.53	0.57
25:X:68:LYS:HB3	25:X:91:LEU:HD22	1.86	0.57
1:2:1565:C:OP2	8:T:101:ARG:NH1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:x:77:LYS:HG2	29:x:117:GLU:HG2	1.87	0.57
1:2:115:U:OP1	1:2:382:C:O2'	2.21	0.57
17:H:129:ILE:O	17:H:133:LEU:HB2	2.05	0.57
14:C:251:LEU:HD12	23:V:23:ILE:HG13	1.85	0.57
8:T:28:LEU:HA	8:T:110:LEU:HD21	1.87	0.57
24:W:44:HIS:NE2	24:W:112:ASP:OD2	2.37	0.57
1:2:1616:U:O4	4:P:40:ARG:NH2	2.37	0.56
14:C:131:GLY:HA3	14:C:216:MET:HB3	1.86	0.56
32:w:327:LEU:HG	32:w:356:VAL:HG22	1.85	0.56
34:K:1024:LEU:HD12	34:K:1032:LEU:HD11	1.87	0.56
1:2:1245:G:C5	1:2:1255:G:N2	2.74	0.56
31:u:285:VAL:HA	31:u:299:MET:HE3	1.86	0.56
31:u:600:ARG:HD3	31:u:646:ALA:HA	1.87	0.56
1:2:1722:G:O6	1:2:1812:U:O2	2.23	0.56
1:2:124:U:OP1	16:G:201:LYS:NZ	2.37	0.56
1:2:913:A:H1'	17:H:66:VAL:HB	1.86	0.56
30:y:9:ALA:HA	30:y:235:LEU:HB2	1.87	0.56
1:2:552:G:OP1	28:e:39:ASN:ND2	2.39	0.56
34:K:377:TYR:HB2	34:K:390:TRP:HH2	1.71	0.56
1:2:816:A:OP2	19:J:10:ARG:NH2	2.38	0.56
4:P:29:SER:OG	4:P:32:GLN:OE1	2.23	0.56
31:u:537:ARG:NH1	31:u:661:PRO:O	2.39	0.56
34:K:838:LYS:O	34:K:841:LEU:HB3	2.05	0.56
1:2:1606:G:H5'	8:T:86:GLY:HA2	1.88	0.56
5:Q:54:PRO:O	5:Q:58:LEU:HB2	2.05	0.56
1:2:1456:G:H1'	34:K:711:ARG:HD2	1.88	0.56
6:R:77:GLU:HA	6:R:80:ARG:HG2	1.88	0.56
1:2:1143:A:H5'	14:C:190:SER:HB3	1.88	0.56
1:2:1398:G:N1	1:2:1448:A:H2	1.99	0.56
1:2:1636:G:H1'	2:F:164:ARG:HH12	1.71	0.56
7:S:104:ASP:OD2	7:S:108:ARG:NH1	2.38	0.56
1:2:1611:G:H4'	7:S:86:ARG:HH21	1.71	0.55
29:x:183:ILE:HB	29:x:204:LEU:HD21	1.89	0.55
1:2:94:G:HO2'	1:2:508:A:HO2'	1.53	0.55
1:2:1095:C:N3	1:2:1149:A:N1	2.53	0.55
16:G:23:LYS:HD3	16:G:41:LEU:HD12	1.89	0.55
16:G:216:ARG:NH1	16:G:219:GLU:OE2	2.34	0.55
31:u:286:ASN:ND2	31:u:348:ASP:OD1	2.39	0.55
17:H:47:ALA:HB3	17:H:63:PHE:HB2	1.86	0.55
18:I:154:LYS:O	18:I:157:LYS:NZ	2.38	0.55
2:F:140:ASP:HB2	10:c:46:VAL:HG12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:81:ARG:NH2	4:P:117:GLY:O	2.40	0.55
1:2:421:G:H5'	20:L:98:LYS:HG3	1.89	0.55
22:O:103:ASN:OD1	22:O:139:SER:OG	2.25	0.55
1:2:1144:A:H2'	1:2:1145:A:C8	2.40	0.55
1:2:1284:A:O4'	1:2:1312:G:N2	2.39	0.55
34:K:1021:LYS:O	34:K:1029:HIS:NE2	2.39	0.55
1:2:1563:G:H5''	8:T:121:ARG:HH21	1.72	0.55
19:J:170:PRO:O	19:J:175:ARG:NH1	2.40	0.55
31:u:157:LEU:HD11	31:u:232:LEU:HD21	1.87	0.55
1:2:382:C:H2'	1:2:383:G:H8	1.72	0.55
1:2:1049:A:H61	33:t:438:ARG:HH12	1.54	0.55
1:2:1607:A:N6	1:2:1632:G:O2'	2.38	0.55
1:2:1256:G:H21	1:2:1659:U:H5'	1.73	0.54
5:Q:19:ALA:HB2	5:Q:75:GLY:HA3	1.89	0.54
21:N:99:ARG:NH1	21:N:143:SER:OG	2.40	0.54
1:2:1398:G:O6	1:2:1448:A:N1	2.40	0.54
8:T:98:SER:OG	8:T:101:ARG:NH2	2.39	0.54
25:X:101:LEU:HB3	25:X:124:LYS:HB2	1.89	0.54
34:K:377:TYR:HB2	34:K:390:TRP:CH2	2.42	0.54
24:W:101:PHE:O	24:W:128:PHE:CA	2.33	0.54
30:y:267:ILE:HD11	30:y:308:MET:HE3	1.90	0.54
1:2:1005:G:OP2	13:B:162:ARG:NH2	2.41	0.54
1:2:1257:G:H4'	1:2:1258:A:H5'	1.90	0.54
4:P:53:GLN:NE2	4:P:82:ASP:OD1	2.39	0.54
6:R:44:LYS:HG2	6:R:47:ARG:HH22	1.72	0.54
18:I:103:LEU:HD22	18:I:170:LYS:HB3	1.88	0.54
1:2:1845:A:H2'	1:2:1846:G:C8	2.43	0.54
12:A:77:ILE:HG12	12:A:99:ILE:HB	1.89	0.54
30:y:10:ASP:HB2	30:y:236:THR:HG22	1.90	0.54
32:w:328:LYS:HE3	33:t:267:TYR:HD1	1.73	0.54
1:2:656:G:O2'	14:C:227:ARG:NH1	2.41	0.54
31:u:272:LEU:HB2	31:u:565:VAL:HG11	1.90	0.54
31:u:667:LEU:HB2	31:u:680:ALA:HB3	1.90	0.53
1:2:913:A:H2	17:H:99:ARG:H	1.55	0.53
1:2:1725:U:H2'	1:2:1726:G:H8	1.73	0.53
15:E:162:ILE:HG22	15:E:169:ILE:HA	1.90	0.53
31:u:294:TYR:OH	31:u:572:CYS:SG	2.66	0.53
15:E:139:LEU:HD11	15:E:169:ILE:HD11	1.89	0.53
1:2:1124:C:H5''	13:B:150:ILE:HG12	1.90	0.53
34:K:716:THR:O	34:K:720:TYR:HB2	2.08	0.53
1:2:587:A:H5'	1:2:592:C:H41	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:N:91:LEU:HD12	21:N:125:LEU:HD12	1.90	0.53
1:2:1748:G:H1	1:2:1786:U:H3	1.56	0.53
13:B:47:THR:OG1	13:B:65:ARG:NH1	2.42	0.53
18:I:205:ARG:O	18:I:205:ARG:NH1	2.42	0.53
22:O:86:LYS:HE3	22:O:124:MET:HE2	1.91	0.53
30:y:13:ALA:HB2	30:y:235:LEU:HB3	1.90	0.53
1:2:1478:U:OP1	34:K:874:ARG:NH1	2.42	0.53
13:B:62:LEU:HD11	13:B:91:VAL:HG22	1.90	0.53
24:W:3:ARG:HD3	24:W:6:VAL:HG12	1.91	0.53
25:X:52:LEU:HD11	25:X:73:GLN:HB2	1.91	0.53
1:2:1471:C:N3	34:K:711:ARG:NH1	2.57	0.53
18:I:89:GLU:HA	18:I:92:ARG:HD2	1.90	0.53
1:2:1610:G:N2	7:S:85:ASN:OD1	2.42	0.52
4:P:37:TYR:O	4:P:42:ARG:NH1	2.42	0.52
6:R:54:VAL:HA	6:R:57:LEU:HG	1.92	0.52
34:K:986:MET:HA	34:K:989:ILE:HG12	1.92	0.52
7:S:30:ILE:HG22	7:S:36:VAL:HG11	1.92	0.52
27:b:38:PRO:HD3	27:b:77:CYS:HA	1.90	0.52
1:2:1584:G:OP1	8:T:77:LYS:NZ	2.38	0.52
23:V:21:ASN:HB3	24:W:67:GLY:HA3	1.92	0.52
31:u:162:PRO:HA	31:u:207:LEU:HD11	1.90	0.52
31:u:171:ASP:OD1	31:u:214:ARG:NH1	2.42	0.52
32:w:181:VAL:HG22	33:t:298:LEU:HD11	1.91	0.52
34:K:112:ARG:HH21	34:K:126:ALA:HB2	1.75	0.52
1:2:1228:A:H2'	1:2:1229:G:C8	2.45	0.52
16:G:49:VAL:HB	16:G:115:LYS:HB3	1.92	0.52
6:R:62:GLN:HB3	34:K:620:TRP:HZ3	1.75	0.52
12:A:173:LEU:HD11	12:A:177:MET:HE3	1.92	0.52
16:G:219:GLU:HA	16:G:222:GLU:HG3	1.92	0.52
13:B:88:THR:HA	13:B:98:THR:HA	1.90	0.52
31:u:94:ILE:HD11	31:u:161:ASP:HA	1.92	0.52
33:t:251:ARG:HH21	33:t:252:ARG:HH21	1.55	0.52
1:2:1195:A:H2'	1:2:1196:A:C8	2.45	0.52
7:S:28:PHE:HA	7:S:31:THR:HB	1.92	0.52
30:y:34:VAL:O	30:y:43:ARG:NH1	2.43	0.52
1:2:1528:G:O2'	1:2:1666:C:OP1	2.27	0.52
32:w:390:LYS:HA	32:w:393:LEU:HD12	1.91	0.52
32:w:410:HIS:O	32:w:414:SER:OG	2.25	0.52
34:K:633:PRO:HB2	34:K:636:VAL:HB	1.92	0.52
1:2:521:A:OP1	19:J:45:ARG:NH1	2.40	0.51
3:M:42:LEU:O	3:M:45:ARG:NH1	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S:3:LEU:N	9:Z:90:GLU:OE1	2.43	0.51
17:H:147:LYS:HE2	17:H:153:LEU:HD22	1.92	0.51
31:u:597:VAL:HG12	31:u:651:VAL:HG22	1.91	0.51
1:2:28:U:H2'	1:2:29:G:H8	1.75	0.51
1:2:617:G:H4'	25:X:88:ASP:HB3	1.92	0.51
11:f:100:LEU:HB3	11:f:103:LEU:HD13	1.91	0.51
14:C:108:LYS:HE2	14:C:233:LEU:HD13	1.93	0.51
34:K:539:VAL:HG22	34:K:547:VAL:HG21	1.92	0.51
7:S:26:ILE:HD11	7:S:52:LEU:HA	1.93	0.51
15:E:206:ASP:HB2	15:E:222:LEU:HD23	1.92	0.51
18:I:142:SER:HB2	18:I:145:ILE:HD12	1.91	0.51
24:W:87:GLU:OE1	24:W:90:GLN:NE2	2.43	0.51
9:Z:50:PHE:HZ	9:Z:87:ALA:HB2	1.74	0.51
34:K:1037:LYS:O	34:K:1041:ARG:N	2.43	0.51
20:L:18:GLN:HB2	20:L:33:LEU:HD22	1.92	0.51
1:2:1473:G:N2	1:2:1476:A:OP2	2.37	0.51
1:2:1726:G:H2'	1:2:1727:G:H8	1.76	0.51
29:x:142:LEU:HD12	29:x:160:LEU:HD21	1.91	0.51
34:K:386:PRO:O	34:K:390:TRP:HB2	2.10	0.51
31:u:612:GLU:OE2	31:u:669:LYS:NZ	2.38	0.51
1:2:1276:A:H61	1:2:1321:G:H1	1.58	0.51
4:P:40:ARG:HH21	4:P:43:ARG:HD3	1.75	0.51
1:2:747:U:O2'	17:H:109:ARG:NE	2.42	0.51
1:2:798:G:H4'	17:H:108:SER:HB2	1.91	0.51
18:I:48:VAL:HG11	18:I:54:LYS:HD2	1.93	0.51
18:I:19:LYS:HD2	18:I:20:PRO:HD2	1.94	0.51
19:J:136:ARG:HE	19:J:158:ASP:HB3	1.75	0.51
20:L:104:LYS:O	25:X:11:ARG:NH2	2.44	0.51
1:2:107:A:H2'	1:2:108:G:C8	2.46	0.50
4:P:64:LYS:NZ	4:P:88:GLU:O	2.44	0.50
27:b:34:ASP:O	27:b:79:PHE:HA	2.12	0.50
1:2:1653:U:H3	1:2:1671:G:H1	1.58	0.50
2:F:167:LYS:NZ	2:F:171:GLU:OE2	2.37	0.50
6:R:66:VAL:HG11	34:K:618:LEU:CD2	2.41	0.50
34:K:131:VAL:HG22	34:K:135:ILE:HG13	1.93	0.50
1:2:69:C:OP2	16:G:164:LYS:NZ	2.41	0.50
1:2:1300:U:OP1	4:P:52:LYS:NZ	2.45	0.50
16:G:2:LYS:O	16:G:108:VAL:HA	2.11	0.50
18:I:69:SER:OG	18:I:191:GLU:OE1	2.27	0.50
31:u:258:VAL:HG22	31:u:274:ILE:HG22	1.92	0.50
1:2:1849:G:OP1	33:t:448:ASN:ND2	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:y:234:CYS:HB2	30:y:252:VAL:HG23	1.92	0.50
1:2:1531:A:H4'	1:2:1605:G:H4'	1.93	0.50
1:2:1536:G:H2'	1:2:1537:A:C8	2.47	0.50
1:2:1810:U:H4'	31:u:56:ARG:HE	1.77	0.50
5:Q:43:GLU:HA	5:Q:45:ARG:HH11	1.76	0.50
24:W:39:THR:HG22	24:W:43:LYS:HE2	1.93	0.50
31:u:155:THR:HG21	31:u:236:LEU:HD22	1.93	0.50
5:Q:58:LEU:HB3	5:Q:62:ARG:HD2	1.94	0.50
22:O:45:THR:HG22	22:O:52:THR:HG22	1.93	0.50
1:2:145:G:H2'	1:2:146:G:C8	2.47	0.50
1:2:1338:G:OP1	34:K:1037:LYS:N	2.41	0.50
7:S:120:HIS:HE1	7:S:124:ARG:HH21	1.58	0.50
13:B:136:ARG:HB2	13:B:218:LEU:HD11	1.92	0.50
17:H:66:VAL:HG22	17:H:96:ALA:HB1	1.94	0.50
32:w:288:LYS:HD3	33:t:266:PHE:HA	1.93	0.50
34:K:378:VAL:O	34:K:379:PRO:C	2.54	0.50
1:2:986:G:OP2	1:2:988:C:N4	2.43	0.49
6:R:87:GLU:HG2	6:R:88:VAL:HG23	1.92	0.49
7:S:39:ARG:HH21	8:T:38:LYS:HB2	1.77	0.49
1:2:552:G:H2'	1:2:553:U:C6	2.47	0.49
12:A:141:ASN:ND2	23:V:31:SER:O	2.36	0.49
29:x:150:LEU:HB3	30:y:361:VAL:HG11	1.93	0.49
32:w:383:LEU:O	32:w:387:GLN:HG2	2.11	0.49
1:2:171:A:H5''	16:G:177:GLN:HG2	1.93	0.49
1:2:524:U:OP1	1:2:525:A:O2'	2.27	0.49
1:2:634:A:OP1	28:e:13:ARG:NH1	2.42	0.49
1:2:1084:A:OP1	1:2:1858:G:O2'	2.25	0.49
32:w:349:LYS:HE2	32:w:388:ARG:HD2	1.95	0.49
1:2:5:U:H2'	1:2:6:G:H8	1.76	0.49
1:2:1786:U:H2'	1:2:1787:G:H8	1.76	0.49
5:Q:51:LEU:HD12	5:Q:52:LEU:HD12	1.94	0.49
34:K:656:ASP:OD1	34:K:656:ASP:N	2.45	0.49
1:2:1037:G:H4'	1:2:1845:A:H4'	1.93	0.49
1:2:1302:G:C2	1:2:1308:U:O4	2.65	0.49
16:G:78:SER:HB3	16:G:92:ARG:HG3	1.95	0.49
21:N:24:THR:O	21:N:27:LYS:NZ	2.44	0.49
31:u:302:ILE:HG22	31:u:560:LEU:HD23	1.94	0.49
34:K:391:LEU:HD11	34:K:434:ALA:HB1	1.94	0.49
1:2:3:C:O2	19:J:18:ARG:NH2	2.46	0.49
17:H:43:LEU:HD22	17:H:68:GLN:HB2	1.95	0.49
31:u:515:ASP:HB3	31:u:518:GLU:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:K:472:PHE:HA	34:K:475:VAL:HG12	1.93	0.49
34:K:928:LEU:HD23	34:K:968:VAL:HG12	1.94	0.49
12:A:42:LYS:HE3	12:A:46:ILE:HB	1.95	0.49
1:2:296:U:O2'	15:E:131:VAL:O	2.25	0.49
1:2:885:U:O2	1:2:901:G:N2	2.38	0.49
12:A:108:PHE:HB2	12:A:136:GLU:HG3	1.95	0.49
13:B:124:HIS:HA	13:B:137:LEU:O	2.13	0.49
18:I:139:LYS:HD3	18:I:141:ARG:HH22	1.77	0.49
29:x:151:ALA:HA	30:y:361:VAL:HG21	1.95	0.49
1:2:4:C:H5'	14:C:230:THR:HG21	1.95	0.49
5:Q:39:LEU:HD12	5:Q:51:LEU:HD13	1.95	0.49
22:O:57:THR:HG23	22:O:60:MET:HE2	1.94	0.49
32:w:213:TRP:CD2	32:w:245:MET:HE3	2.48	0.49
1:2:1345:G:OP2	1:2:1370:A:O2'	2.31	0.48
1:2:816:A:P	19:J:10:ARG:HH22	2.36	0.48
1:2:1032:C:H5''	21:N:109:LYS:HD2	1.95	0.48
1:2:1648:G:N2	1:2:1675:A:OP2	2.38	0.48
4:P:53:GLN:HG3	4:P:83:MET:SD	2.53	0.48
6:R:84:TYR:HB3	12:A:205:ARG:HH12	1.79	0.48
31:u:604:ASN:HD22	31:u:679:ILE:HG22	1.77	0.48
34:K:290:GLN:HB3	34:K:294:LYS:NZ	2.28	0.48
1:2:1253:A:O2'	1:2:1666:C:O2'	2.28	0.48
1:2:1614:A:OP2	4:P:42:ARG:NH2	2.44	0.48
18:I:42:ARG:HB3	18:I:59:ARG:HG2	1.94	0.48
34:K:780:LEU:O	34:K:788:GLN:NE2	2.43	0.48
34:K:865:CYS:HA	34:K:868:GLU:HB2	1.94	0.48
4:P:21:ASP:OD1	4:P:22:LEU:N	2.40	0.48
12:A:29:ASN:HB3	12:A:151:ASP:HB3	1.94	0.48
26:Y:14:THR:HG22	26:Y:21:LYS:HG2	1.95	0.48
1:2:527:C:H2'	1:2:528:A:H8	1.78	0.48
1:2:871:U:H3'	1:2:872:A:H4'	1.95	0.48
1:2:1234:C:H5''	1:2:1246:A:H61	1.79	0.48
1:2:656:G:H5'	1:2:662:G:N2	2.29	0.48
1:2:943:U:H2'	1:2:944:A:C8	2.49	0.48
1:2:1195:A:H2'	1:2:1196:A:H8	1.79	0.48
16:G:135:PRO:HG2	16:G:141:ILE:HD13	1.94	0.48
1:2:508:A:H3'	1:2:509:G:H8	1.78	0.48
1:2:1562:C:H2'	1:2:1563:G:H8	1.78	0.48
19:J:60:LEU:HD22	19:J:70:ARG:HA	1.96	0.48
22:O:142:ARG:NH2	29:x:167:ASP:O	2.47	0.48
1:2:51:U:H2'	1:2:52:G:C8	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:H:93:VAL:HG11	17:H:133:LEU:HD12	1.96	0.48
30:y:282:ARG:NH1	30:y:284:PHE:O	2.45	0.48
34:K:975:VAL:HA	34:K:978:LEU:HB2	1.96	0.48
1:2:997:A:N1	1:2:1032:C:O2'	2.43	0.48
6:R:81:ARG:O	12:A:205:ARG:NH1	2.46	0.48
31:u:731:LEU:HD11	31:u:741:ILE:HG13	1.96	0.48
34:K:377:TYR:O	34:K:378:VAL:C	2.57	0.48
34:K:869:VAL:O	34:K:874:ARG:NH2	2.40	0.48
1:2:507:G:OP2	26:Y:104:ARG:NH2	2.47	0.48
19:J:128:VAL:O	19:J:132:GLN:HG2	2.13	0.48
34:K:315:LEU:HD13	34:K:352:LEU:HD23	1.96	0.48
1:2:483:C:H5''	25:X:48:LYS:HE3	1.96	0.47
1:2:685:A:H1'	24:W:58:ALA:HB2	1.96	0.47
1:2:748:C:H42	1:2:794:A:H61	1.62	0.47
1:2:1220:A:N3	1:2:1677:U:O2'	2.38	0.47
1:2:1376:A:H2	30:y:333:LYS:HD3	1.79	0.47
34:K:304:THR:HA	34:K:307:MET:HE3	1.96	0.47
8:T:77:LYS:HD3	8:T:94:ARG:HH21	1.78	0.47
26:Y:114:MET:HE3	26:Y:122:LYS:HB3	1.95	0.47
1:2:643:A:OP1	19:J:39:ASN:ND2	2.47	0.47
13:B:107:ARG:NH1	22:O:133:THR:O	2.47	0.47
15:E:45:ILE:HG13	15:E:61:VAL:HG21	1.96	0.47
16:G:48:TYR:OH	16:G:119:LYS:O	2.32	0.47
16:G:57:ASP:HA	16:G:106:LEU:HA	1.95	0.47
17:H:109:ARG:HG2	17:H:110:THR:H	1.79	0.47
31:u:285:VAL:HG23	31:u:346:LYS:HE3	1.96	0.47
1:2:1323:U:H2'	1:2:1324:G:O4'	2.13	0.47
3:M:48:HIS:ND1	3:M:112:LYS:O	2.42	0.47
6:R:66:VAL:CG2	34:K:614:ILE:HG23	2.45	0.47
11:f:145:CYS:O	33:t:293:ARG:NH2	2.48	0.47
29:x:116:VAL:HG11	29:x:137:VAL:HG11	1.96	0.47
30:y:18:ALA:HB1	30:y:20:LEU:HD23	1.97	0.47
1:2:980:A:H2'	1:2:981:A:C8	2.49	0.47
1:2:1536:G:H2'	1:2:1537:A:H8	1.77	0.47
18:I:61:ASP:OD1	18:I:61:ASP:N	2.46	0.47
30:y:122:PRO:HB2	30:y:128:PHE:HD2	1.79	0.47
14:C:166:ARG:HB2	14:C:248:TYR:CD1	2.49	0.47
31:u:588:GLU:O	31:u:621:ARG:NH2	2.48	0.47
34:K:201:GLN:HB3	34:K:210:LEU:HD13	1.97	0.47
1:2:1245:G:C6	1:2:1255:G:C2	3.03	0.47
1:2:1656:G:H2'	1:2:1657:G:H8	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:66:VAL:HG21	12:A:185:MET:HB2	1.95	0.47
12:A:82:THR:OG1	30:y:343:ASP:OD2	2.32	0.47
16:G:1:MET:HG2	16:G:24:LEU:HD21	1.95	0.47
16:G:7:PHE:O	16:G:11:GLY:N	2.48	0.47
34:K:290:GLN:HB3	34:K:294:LYS:HZ3	1.80	0.47
34:K:863:ILE:O	34:K:866:THR:OG1	2.25	0.47
9:Z:68:ILE:HB	9:Z:109:TYR:HB2	1.97	0.47
16:G:48:TYR:HE1	16:G:116:LYS:HD2	1.80	0.47
1:2:84:A:N3	1:2:150:A:O2'	2.46	0.47
1:2:1218:C:H1'	1:2:1683:C:H42	1.80	0.47
16:G:85:ARG:O	16:G:87:ARG:NH1	2.48	0.47
1:2:581:U:OP1	19:J:133:ARG:NH2	2.47	0.46
1:2:640:A:H2'	1:2:641:A:C8	2.50	0.46
1:2:1274:G:O6	11:f:89:LYS:NZ	2.48	0.46
7:S:18:THR:HG21	7:S:33:ILE:HG22	1.97	0.46
12:A:108:PHE:HB3	12:A:140:VAL:HG21	1.97	0.46
25:X:105:PHE:HD1	25:X:121:LYS:HB3	1.79	0.46
30:y:268:LEU:HB3	30:y:293:LEU:HB3	1.97	0.46
27:b:42:LYS:HE3	27:b:57:VAL:HB	1.97	0.46
32:w:208:PRO:HA	32:w:245:MET:HE1	1.97	0.46
32:w:240:ASN:O	32:w:242:LYS:NZ	2.45	0.46
34:K:921:ILE:HD11	34:K:950:LEU:HD13	1.97	0.46
30:y:232:VAL:O	30:y:251:HIS:NE2	2.46	0.46
34:K:338:HIS:HB3	34:K:341:VAL:HG22	1.96	0.46
1:2:67:C:N4	16:G:168:LYS:O	2.38	0.46
1:2:948:C:H2'	1:2:949:G:H8	1.80	0.46
1:2:1722:G:O6	1:2:1812:U:C2	2.69	0.46
1:2:1779:G:H2'	1:2:1780:G:C8	2.51	0.46
5:Q:57:LEU:HD21	5:Q:115:TYR:CG	2.51	0.46
25:X:46:HIS:CD2	25:X:103:ALA:HB2	2.51	0.46
26:Y:54:VAL:HG22	26:Y:76:TYR:HB2	1.97	0.46
31:u:286:ASN:HD21	31:u:349:PRO:HD2	1.80	0.46
1:2:1302:G:N2	1:2:1308:U:O4	2.48	0.46
1:2:1758:G:C2	1:2:1775:U:O2	2.68	0.46
6:R:30:THR:HA	6:R:33:ARG:HG2	1.97	0.46
6:R:66:VAL:CG1	34:K:618:LEU:HD21	2.46	0.46
14:C:196:ILE:HB	14:C:223:TYR:HB2	1.95	0.46
31:u:144:HIS:O	31:u:148:ASP:HB2	2.16	0.46
31:u:624:ARG:NH2	31:u:780:ASP:OD2	2.48	0.46
34:K:245:THR:HG21	34:K:310:LEU:HD11	1.97	0.46
1:2:1562:C:H2'	1:2:1563:G:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1821:U:H2'	1:2:1822:A:C8	2.50	0.46
16:G:58:LYS:HA	16:G:107:SER:HB2	1.97	0.46
21:N:30:SER:HB2	21:N:67:THR:HA	1.97	0.46
31:u:627:PRO:HA	31:u:653:THR:O	2.16	0.46
1:2:297:A:H5'	15:E:132:GLY:HA2	1.98	0.46
1:2:1845:A:H2'	1:2:1846:G:H8	1.80	0.46
9:Z:79:ILE:HG23	9:Z:83:LEU:HD23	1.96	0.46
1:2:5:U:H2'	1:2:6:G:C8	2.51	0.46
1:2:1860:A:OP2	29:x:178:ARG:NH2	2.44	0.46
17:H:140:VAL:HG11	17:H:193:GLN:HG3	1.98	0.46
31:u:624:ARG:HD3	31:u:783:VAL:HG22	1.98	0.46
34:K:113:PHE:HD1	34:K:127:VAL:HG21	1.81	0.46
1:2:857:U:H2'	1:2:858:A:C8	2.51	0.46
2:F:32:ASP:OD2	2:F:34:SER:OG	2.26	0.46
5:Q:42:ILE:HG22	5:Q:44:PRO:HD2	1.97	0.46
1:2:12:U:H2'	1:2:13:C:C6	2.51	0.46
1:2:218:U:O2	18:I:184:ARG:NH2	2.37	0.46
1:2:1665:G:C8	8:T:88:MET:HE1	2.51	0.46
2:F:71:ARG:NH2	2:F:148:ASN:OD1	2.35	0.46
31:u:152:VAL:HG21	31:u:254:PHE:HB2	1.98	0.46
1:2:527:C:H4'	19:J:121:LYS:HD2	1.97	0.45
1:2:1047:C:H5''	22:O:143:LYS:HA	1.98	0.45
29:x:202:ILE:HG12	29:x:225:ILE:HD11	1.98	0.45
1:2:115:U:H2'	1:2:116:U:C6	2.51	0.45
1:2:996:A:H2'	1:2:997:A:C8	2.52	0.45
1:2:1337:C:OP1	34:K:1036:ARG:NH2	2.50	0.45
1:2:1781:A:H2'	1:2:1782:G:C8	2.50	0.45
10:c:33:GLU:OE1	10:c:41:SER:OG	2.34	0.45
16:G:102:VAL:HG13	16:G:106:LEU:HD12	1.97	0.45
34:K:535:VAL:HG12	34:K:572:VAL:HG11	1.97	0.45
1:2:492:C:OP2	26:Y:107:ARG:NH2	2.47	0.45
1:2:528:A:H2'	1:2:529:A:H8	1.80	0.45
1:2:1609:C:H3'	7:S:132:ARG:HH12	1.82	0.45
13:B:146:ARG:HD3	13:B:206:PRO:HG3	1.98	0.45
8:T:31:PRO:HG3	8:T:102:ARG:HE	1.82	0.45
8:T:56:ARG:HG2	8:T:103:VAL:HG21	1.99	0.45
16:G:135:PRO:HB3	16:G:144:LEU:HD12	1.97	0.45
18:I:88:ASN:ND2	18:I:205:ARG:HE	2.14	0.45
21:N:110:ASP:OD1	21:N:114:ARG:NH1	2.50	0.45
31:u:89:PRO:HA	31:u:159:LEU:HB2	1.97	0.45
34:K:881:LEU:HB3	34:K:927:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1277:C:H2'	1:2:1278:A:H8	1.82	0.45
3:M:84:LYS:HE3	3:M:88:TRP:HE1	1.81	0.45
14:C:172:ASN:ND2	19:J:95:ASP:OD2	2.36	0.45
26:Y:104:ARG:O	26:Y:108:LYS:HG2	2.16	0.45
32:w:328:LYS:O	32:w:332:MET:HG3	2.17	0.45
1:2:1485:U:H2'	1:2:1486:A:H8	1.81	0.45
1:2:1581:C:H5''	1:2:1582:C:H5	1.82	0.45
1:2:1597:C:H4'	1:2:1603:G:C6	2.51	0.45
2:F:154:LEU:HD22	2:F:177:LEU:HD23	1.99	0.45
14:C:137:VAL:HG21	14:C:244:ILE:HD12	1.99	0.45
24:W:25:VAL:O	24:W:62:VAL:HA	2.16	0.45
1:2:544:G:H2'	1:2:545:A:H8	1.82	0.45
1:2:1511:U:O2'	32:w:271:HIS:NE2	2.50	0.45
14:C:183:LYS:HE2	24:W:95:PRO:HA	1.99	0.45
18:I:3:ILE:O	18:I:30:GLY:N	2.44	0.45
27:b:64:CYS:HB3	27:b:73:LEU:HD23	1.98	0.45
8:T:126:GLN:OE1	8:T:129:ARG:NH1	2.50	0.45
28:e:28:LYS:HD3	28:e:32:ALA:HB1	1.99	0.45
30:y:359:THR:HB	30:y:374:VAL:HG23	1.99	0.45
33:t:252:ARG:NH1	33:t:257:THR:OG1	2.50	0.45
34:K:1037:LYS:HA	34:K:1040:ALA:HB3	1.99	0.45
1:2:1310:U:H5''	3:M:40:LYS:HZ3	1.82	0.45
16:G:7:PHE:O	16:G:11:GLY:CA	2.65	0.45
27:b:54:VAL:HG13	27:b:63:LEU:HB2	1.99	0.45
32:w:293:PRO:HA	32:w:296:GLU:HG2	1.98	0.45
12:A:5:LEU:HD21	23:V:41:LYS:HA	1.99	0.44
15:E:107:GLY:HA2	15:E:189:LEU:HD22	2.00	0.44
31:u:155:THR:HA	31:u:184:THR:O	2.16	0.44
33:t:292:ASN:OD1	33:t:293:ARG:N	2.49	0.44
1:2:223:C:H2'	1:2:224:A:C8	2.52	0.44
1:2:661:U:OP2	25:X:3:LYS:NZ	2.46	0.44
1:2:1726:G:H2'	1:2:1727:G:C8	2.51	0.44
6:R:27:ASP:HB3	6:R:30:THR:HG22	1.98	0.44
11:f:81:LYS:HD2	31:u:487:GLU:HB3	1.99	0.44
12:A:109:THR:N	12:A:136:GLU:OE2	2.50	0.44
15:E:45:ILE:HD12	15:E:80:ILE:HD12	1.99	0.44
31:u:525:ALA:HB2	33:t:362:ASN:HB2	1.99	0.44
34:K:410:LEU:HD23	34:K:413:LEU:HD12	1.99	0.44
34:K:840:LEU:HA	34:K:843:ILE:HG12	2.00	0.44
1:2:792:C:H2'	1:2:793:G:H8	1.82	0.44
1:2:1100:A:H5'	30:y:320:ARG:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:u:124:LEU:HB3	31:u:133:TRP:HB2	1.99	0.44
34:K:643:LEU:HB3	34:K:647:LEU:HD23	2.00	0.44
1:2:528:A:H2'	1:2:529:A:C8	2.53	0.44
1:2:1588:A:H2'	1:2:1589:A:C8	2.52	0.44
1:2:1725:U:H2'	1:2:1726:G:C8	2.51	0.44
16:G:7:PHE:O	16:G:11:GLY:HA2	2.18	0.44
18:I:57:ALA:HB2	18:I:183:GLY:HA2	2.00	0.44
21:N:5:HIS:CE1	21:N:121:ARG:HG3	2.53	0.44
32:w:248:ARG:HA	32:w:248:ARG:HD3	1.76	0.44
12:A:134:LEU:HD22	12:A:144:THR:HG21	1.98	0.44
14:C:166:ARG:HB3	14:C:247:THR:HB	1.99	0.44
18:I:84:ASN:ND2	18:I:90:LEU:HD23	2.32	0.44
31:u:91:HIS:HB3	31:u:94:ILE:HG12	1.99	0.44
1:2:1605:G:OP1	8:T:84:ARG:NH2	2.44	0.44
1:2:1606:G:H22	1:2:1632:G:H2'	1.82	0.44
1:2:1652:G:H1	1:2:1672:U:H3	1.66	0.44
8:T:77:LYS:HA	8:T:94:ARG:HG2	2.00	0.44
18:I:4:SER:OG	18:I:6:ASP:OD2	2.27	0.44
20:L:85:THR:HG22	20:L:112:HIS:HA	1.99	0.44
1:2:546:G:H2'	1:2:547:G:H3'	1.99	0.44
3:M:69:CYS:HA	3:M:74:ILE:HB	2.00	0.44
30:y:66:VAL:HA	30:y:69:PHE:CE2	2.53	0.44
34:K:1017:PHE:HZ	34:K:1033:VAL:HG12	1.82	0.44
1:2:520:A:H5''	19:J:12:THR:HG23	1.99	0.44
1:2:1285:G:H1	3:M:56:CYS:HA	1.83	0.44
1:2:1785:C:O2'	1:2:1786:U:O4'	2.36	0.44
1:2:495:U:OP1	15:E:49:ARG:NH1	2.51	0.44
2:F:102:LEU:HB2	9:Z:67:LEU:HD12	1.99	0.44
5:Q:43:GLU:HG3	5:Q:44:PRO:HD3	2.00	0.44
12:A:76:VAL:HG12	12:A:87:VAL:HG13	2.00	0.44
17:H:101:LEU:O	17:H:116:ARG:NH1	2.51	0.44
32:w:208:PRO:HB2	32:w:240:ASN:HD22	1.83	0.44
1:2:145:G:O6	16:G:178:ARG:NH2	2.49	0.43
1:2:168:C:O2'	16:G:132:ARG:O	2.29	0.43
1:2:561:A:H2'	1:2:562:U:O4'	2.18	0.43
1:2:1065:G:OP1	22:O:149:ARG:NH2	2.51	0.43
1:2:1331:C:H2'	1:2:1332:A:H8	1.82	0.43
12:A:217:ALA:O	30:y:64:ARG:NH2	2.51	0.43
31:u:251:ALA:HB3	31:u:583:SER:OG	2.18	0.43
31:u:399:SER:HA	31:u:402:ALA:HB3	2.00	0.43
32:w:354:TYR:HD2	33:t:252:ARG:HD3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:388:U:H2'	1:2:389:A:C8	2.53	0.43
1:2:1154:U:OP2	14:C:187:ARG:NH2	2.40	0.43
18:I:119:LEU:HD11	18:I:153:LYS:HG2	2.00	0.43
30:y:234:CYS:HB3	30:y:236:THR:HG23	2.00	0.43
1:2:28:U:H2'	1:2:29:G:C8	2.54	0.43
1:2:615:C:H4'	28:e:6:LEU:HD21	2.00	0.43
11:f:137:ASP:OD1	11:f:137:ASP:N	2.51	0.43
34:K:909:GLY:HA2	34:K:916:MET:HE1	1.99	0.43
1:2:1054:G:H2'	1:2:1055:A:C8	2.54	0.43
1:2:1102:G:OP2	13:B:151:ARG:NH1	2.50	0.43
1:2:1542:C:H5''	8:T:62:ARG:HH22	1.83	0.43
12:A:142:LEU:O	23:V:60:ARG:NH2	2.51	0.43
31:u:596:MET:O	31:u:651:VAL:HA	2.19	0.43
34:K:214:LEU:HD22	34:K:241:LEU:HD13	2.01	0.43
1:2:1217:A:H2'	1:2:1218:C:C6	2.54	0.43
1:2:1375:G:H2'	1:2:1376:A:C8	2.53	0.43
6:R:70:SER:HA	34:K:614:ILE:HD11	2.01	0.43
6:R:84:TYR:HB3	12:A:205:ARG:NH1	2.34	0.43
7:S:81:ASP:OD1	7:S:81:ASP:N	2.52	0.43
14:C:107:LEU:HD22	14:C:209:VAL:HG13	2.00	0.43
24:W:49:GLU:O	24:W:64:ASN:ND2	2.52	0.43
25:X:17:ARG:O	25:X:21:LYS:HB2	2.18	0.43
30:y:129:HIS:NE2	30:y:131:PRO:HD2	2.32	0.43
31:u:113:LEU:HD23	31:u:122:PHE:HB3	2.01	0.43
33:t:434:ILE:O	33:t:438:ARG:HG3	2.18	0.43
2:F:155:CYS:O	2:F:159:ARG:HG3	2.18	0.43
18:I:105:ASP:OD1	18:I:106:SER:N	2.47	0.43
30:y:117:GLN:HE22	30:y:123:LEU:HD11	1.84	0.43
34:K:880:LEU:HG	34:K:884:MET:HE1	2.00	0.43
1:2:649:U:H2'	1:2:650:A:C8	2.54	0.43
1:2:1033:G:N1	1:2:1080:A:O2'	2.40	0.43
12:A:143:PRO:HG3	23:V:32:ILE:HG23	2.01	0.43
30:y:65:LEU:HA	30:y:68:GLU:CD	2.44	0.43
31:u:290:HIS:HA	31:u:296:ASP:HA	2.00	0.43
1:2:819:G:OP1	19:J:79:ARG:NH2	2.38	0.43
15:E:31:PRO:HG2	15:E:38:LEU:HB2	2.00	0.43
29:x:200:THR:HG22	29:x:213:GLY:HA3	2.01	0.43
30:y:28:TYR:HE1	30:y:54:ARG:HH11	1.67	0.43
1:2:17:C:H2'	1:2:18:C:C6	2.53	0.43
1:2:1226:G:N1	1:2:1639:G:OP2	2.41	0.43
19:J:110:LEU:HB2	19:J:147:PHE:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:105:LEU:HG	13:B:213:ARG:HA	2.01	0.43
14:C:65:LYS:HD2	14:C:273:LEU:HD13	1.99	0.43
26:Y:58:PHE:HE1	26:Y:74:MET:HE2	1.84	0.43
31:u:299:MET:HB3	31:u:562:VAL:HG12	2.01	0.43
1:2:672:A:N6	1:2:1027:A:OP1	2.47	0.42
1:2:1285:G:H5'	3:M:35:ILE:HB	2.01	0.42
1:2:1291:A:O2'	11:f:140:TYR:OH	2.25	0.42
1:2:1375:G:H2'	1:2:1376:A:H8	1.83	0.42
1:2:1533:A:H5'	1:2:1637:A:H62	1.84	0.42
15:E:152:PRO:HG2	16:G:216:ARG:HG3	2.01	0.42
31:u:208:SER:O	31:u:212:GLU:HG3	2.19	0.42
34:K:201:GLN:OE1	34:K:204:SER:OG	2.36	0.42
34:K:353:PHE:HD1	34:K:400:ASN:HD22	1.67	0.42
34:K:725:ASP:OD1	34:K:725:ASP:N	2.52	0.42
10:c:68:LEU:HD11	29:x:155:LEU:HD22	2.01	0.42
14:C:66:LEU:HD11	14:C:81:ILE:HG12	2.00	0.42
30:y:365:ASP:OD1	30:y:365:ASP:N	2.42	0.42
1:2:114:G:H5'	20:L:132:ARG:HD3	2.01	0.42
1:2:118:C:H1'	1:2:445:A:C5	2.54	0.42
1:2:604:A:N3	1:2:639:C:O2'	2.49	0.42
1:2:748:C:N4	1:2:794:A:H61	2.17	0.42
1:2:1236:G:N2	1:2:1522:A:H62	2.12	0.42
19:J:94:LEU:HD12	19:J:97:ILE:HD12	2.00	0.42
25:X:84:PHE:CE2	25:X:86:PRO:HA	2.54	0.42
30:y:354:LYS:HE3	30:y:377:ASP:HA	2.01	0.42
1:2:494:C:N4	1:2:509:G:H21	2.16	0.42
1:2:1189:A:H2'	1:2:1190:A:C8	2.54	0.42
12:A:145:ILE:HG12	12:A:159:ILE:HB	2.00	0.42
31:u:510:ARG:HH12	31:u:633:THR:HG21	1.84	0.42
34:K:901:CYS:HA	34:K:904:VAL:HG22	2.00	0.42
1:2:49:C:H2'	1:2:472:C:H41	1.84	0.42
1:2:594:A:H61	1:2:643:A:H5''	1.84	0.42
1:2:1293:A:H1'	11:f:138:ARG:HH21	1.85	0.42
13:B:228:LEU:HD12	13:B:228:LEU:HA	1.92	0.42
14:C:271:ASP:OD1	14:C:271:ASP:N	2.51	0.42
16:G:113:ILE:HD13	16:G:113:ILE:HG21	1.89	0.42
21:N:78:LYS:HE2	21:N:78:LYS:HB2	1.73	0.42
24:W:27:ILE:HG13	24:W:61:ILE:HB	2.01	0.42
31:u:616:PHE:O	31:u:622:ARG:HA	2.20	0.42
34:K:151:LEU:HB3	34:K:155:MET:HE2	2.02	0.42
34:K:889:LEU:HD22	34:K:895:GLN:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:808:A:O2'	1:2:809:A:H8	2.02	0.42
1:2:1648:G:H5'	5:Q:125:ARG:HB2	2.01	0.42
31:u:248:ASP:O	31:u:281:GLN:NE2	2.45	0.42
1:2:453:C:O2'	16:G:92:ARG:O	2.36	0.42
1:2:1213:C:H2'	1:2:1214:A:C8	2.54	0.42
2:F:47:LYS:NZ	5:Q:115:TYR:O	2.53	0.42
9:Z:65:TYR:O	9:Z:67:LEU:N	2.52	0.42
12:A:188:THR:HG23	12:A:189:ILE:HG13	2.00	0.42
19:J:140:GLN:NE2	26:Y:64:PHE:O	2.45	0.42
34:K:859:ILE:O	34:K:863:ILE:HG13	2.19	0.42
1:2:102:A:H5'	1:2:104:A:C4	2.55	0.42
26:Y:114:MET:HA	26:Y:117:VAL:HG22	2.02	0.42
31:u:144:HIS:CE1	31:u:622:ARG:HH22	2.37	0.42
31:u:624:ARG:NE	31:u:782:TYR:O	2.53	0.42
32:w:326:MET:HA	32:w:329:ILE:HG22	2.02	0.42
34:K:1018:GLU:HB3	34:K:1022:ARG:NH1	2.34	0.42
1:2:1101:U:H2'	1:2:1102:G:C8	2.54	0.42
1:2:1786:U:H2'	1:2:1787:G:C8	2.53	0.42
31:u:258:VAL:HG21	31:u:579:LEU:HD12	2.02	0.42
1:2:610:G:OP1	11:f:77:ALA:N	2.52	0.42
1:2:867:G:H2'	1:2:868:G:C8	2.54	0.42
19:J:28:GLU:OE2	19:J:44:TRP:NE1	2.42	0.42
31:u:151:LYS:HB3	31:u:180:GLN:HE22	1.84	0.42
1:2:65:C:H4'	16:G:172:LYS:HD3	2.02	0.41
1:2:1485:U:H2'	1:2:1486:A:C8	2.55	0.41
1:2:67:C:H5''	16:G:162:LEU:HD21	2.01	0.41
6:R:76:GLU:OE2	6:R:77:GLU:HG3	2.20	0.41
13:B:25:PHE:HA	13:B:28:LYS:HG3	2.00	0.41
19:J:138:ARG:HG3	19:J:139:LYS:H	1.85	0.41
20:L:91:ASP:HB3	20:L:104:LYS:HE2	2.02	0.41
26:Y:6:THR:HB	26:Y:28:LEU:HB2	2.01	0.41
34:K:888:PHE:HD2	34:K:902:TYR:HB2	1.85	0.41
34:K:1030:ARG:O	34:K:1033:VAL:HG22	2.20	0.41
1:2:29:G:H2'	1:2:30:C:C6	2.55	0.41
1:2:1470:C:H2'	1:2:1471:C:H6	1.86	0.41
19:J:87:LEU:HD23	19:J:91:LYS:HZ2	1.86	0.41
1:2:1010:G:H2'	1:2:1011:A:H8	1.85	0.41
1:2:1486:A:H2'	1:2:1487:A:C8	2.55	0.41
4:P:98:ASN:HB3	4:P:120:SER:HB3	2.01	0.41
6:R:98:VAL:HG21	6:R:117:LEU:HG	2.02	0.41
15:E:128:LYS:HG2	15:E:140:VAL:HB	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:885:U:H3	1:2:901:G:H1	1.68	0.41
1:2:1871:C:O2	29:x:114:ARG:NH2	2.49	0.41
2:F:49:LEU:HD12	5:Q:50:LYS:HG2	2.02	0.41
10:c:12:ALA:HB1	10:c:32:VAL:HG13	2.01	0.41
32:w:334:TYR:CG	32:w:367:PHE:HZ	2.38	0.41
33:t:311:LYS:HE3	33:t:311:LYS:HB2	1.83	0.41
34:K:113:PHE:HB2	34:K:127:VAL:HG11	2.02	0.41
34:K:182:VAL:O	34:K:186:LYS:HG3	2.21	0.41
34:K:253:ARG:HD2	34:K:306:HIS:CG	2.56	0.41
1:2:303:C:O2	18:I:184:ARG:NH1	2.53	0.41
1:2:1472:C:O2	34:K:711:ARG:NH2	2.54	0.41
1:2:1781:A:H2'	1:2:1782:G:H8	1.86	0.41
1:2:1866:A:H5''	30:y:392:LEU:HD21	2.03	0.41
30:y:80:SER:OG	30:y:83:ASP:OD2	2.34	0.41
32:w:342:LEU:HD11	32:w:360:LEU:HD21	2.03	0.41
34:K:210:LEU:HA	34:K:213:VAL:HG12	2.03	0.41
1:2:982:G:H21	1:2:1045:U:H1'	1.85	0.41
1:2:991:G:C2	30:y:407:LYS:HA	2.56	0.41
1:2:1692:U:H2'	1:2:1693:G:C8	2.56	0.41
4:P:22:LEU:HA	4:P:25:LEU:HD12	2.02	0.41
30:y:294:LYS:HD3	30:y:316:VAL:HG12	2.01	0.41
34:K:264:LEU:HD23	34:K:264:LEU:HA	1.91	0.41
2:F:30:ILE:HG21	2:F:36:GLN:HA	2.02	0.41
11:f:126:CYS:HB2	11:f:130:VAL:HG21	2.01	0.41
14:C:165:VAL:HG11	14:C:217:ALA:HB1	2.02	0.41
17:H:61:ILE:HD11	17:H:176:VAL:HG11	2.03	0.41
1:2:641:A:OP1	19:J:40:LYS:NZ	2.37	0.41
1:2:674:C:H2'	1:2:675:U:C6	2.56	0.41
1:2:929:G:H2'	1:2:930:C:O4'	2.21	0.41
1:2:973:C:O2	22:O:55:ARG:NH2	2.54	0.41
1:2:1535:U:O2'	2:F:81:ARG:NH1	2.54	0.41
1:2:1736:G:H2'	1:2:1737:G:C8	2.56	0.41
2:F:68:ILE:HD11	2:F:151:ILE:HD11	2.02	0.41
13:B:142:PHE:O	13:B:208:HIS:N	2.47	0.41
14:C:246:LYS:HA	14:C:249:SER:HB2	2.02	0.41
21:N:83:ASP:OD1	21:N:84:LEU:N	2.53	0.41
32:w:305:ALA:HB2	32:w:337:ALA:HB1	2.03	0.41
32:w:402:LEU:HD22	32:w:421:LEU:HD13	2.02	0.41
34:K:407:ASP:OD1	34:K:407:ASP:N	2.53	0.41
34:K:638:ILE:O	34:K:641:LYS:NZ	2.54	0.41
1:2:57:U:OP1	1:2:504:G:O2'	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:75:G:H1	16:G:155:GLN:HA	1.86	0.41
7:S:38:ARG:O	7:S:42:HIS:ND1	2.54	0.41
16:G:50:VAL:HG22	16:G:113:ILE:HG22	2.03	0.41
16:G:56:ASN:HB2	16:G:108:VAL:HG12	2.02	0.41
1:2:747:U:H2'	1:2:748:C:C6	2.56	0.40
1:2:1139:C:H2'	1:2:1140:G:O4'	2.21	0.40
5:Q:34:VAL:HG12	5:Q:39:LEU:HD22	2.02	0.40
6:R:69:ILE:H	6:R:69:ILE:HG12	1.73	0.40
19:J:60:LEU:HD11	19:J:73:GLU:HG2	2.03	0.40
22:O:56:VAL:HA	22:O:60:MET:HE3	2.03	0.40
34:K:223:LYS:HD3	34:K:223:LYS:HA	1.89	0.40
1:2:1154:U:H2'	14:C:192:LEU:HD11	2.03	0.40
1:2:1222:G:H2'	1:2:1223:A:C8	2.56	0.40
1:2:1325:G:O2'	1:2:1327:G:OP2	2.36	0.40
4:P:31:GLU:OE2	4:P:32:GLN:NE2	2.54	0.40
19:J:88:ASP:HB2	19:J:91:LYS:HG2	2.02	0.40
20:L:35:ARG:HH21	20:L:53:GLY:C	2.30	0.40
20:L:127:THR:HB	20:L:144:LYS:HG2	2.03	0.40
34:K:171:LEU:O	34:K:175:LEU:HB2	2.21	0.40
1:2:808:A:H5''	15:E:219:ALA:O	2.21	0.40
1:2:1333:U:H3	1:2:1495:G:H1	1.69	0.40
1:2:1748:G:H2'	1:2:1749:G:H8	1.87	0.40
1:2:1798:C:H2'	1:2:1799:G:O4'	2.21	0.40
2:F:100:ILE:HA	2:F:178:ILE:HD11	2.04	0.40
3:M:51:VAL:HG22	3:M:77:ILE:HB	2.03	0.40
7:S:40:TYR:CZ	7:S:97:GLN:HG2	2.56	0.40
7:S:79:ILE:HA	7:S:80:PRO:HD3	1.94	0.40
12:A:10:MET:HB2	12:A:55:TRP:CD1	2.55	0.40
12:A:151:ASP:OD1	12:A:151:ASP:N	2.53	0.40
27:b:59:CYS:SG	27:b:61:THR:OG1	2.71	0.40
1:2:218:U:H2'	1:2:219:U:C6	2.56	0.40
1:2:1545:A:H2'	1:2:1546:G:C8	2.56	0.40
1:2:1609:C:H5''	7:S:132:ARG:HH11	1.86	0.40
14:C:221:ASP:OD1	14:C:221:ASP:N	2.54	0.40
15:E:126:VAL:HG21	15:E:139:LEU:HD22	2.02	0.40
16:G:2:LYS:HD3	16:G:15:LEU:HD21	2.03	0.40
22:O:54:CYS:SG	22:O:81:VAL:HG22	2.62	0.40
31:u:596:MET:HG2	31:u:665:VAL:HG11	2.02	0.40
32:w:329:ILE:HD11	32:w:338:ASN:ND2	2.37	0.40
5:Q:117:ARG:NH1	5:Q:123:ASP:OD1	2.41	0.40
7:S:73:ASN:H	7:S:73:ASN:HD22	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:E:181:CYS:HB3	15:E:195:ILE:HD11	2.03	0.40
18:I:174:CYS:HB2	18:I:190:LEU:HD21	2.04	0.40
22:O:149:ARG:HE	22:O:150:ARG:H	1.69	0.40
31:u:272:LEU:HB3	31:u:562:VAL:HG22	2.02	0.40
34:K:620:TRP:HD1	34:K:657:LEU:HD23	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	187/204 (92%)	178 (95%)	9 (5%)	0	100	100
3	M	121/132 (92%)	113 (93%)	8 (7%)	0	100	100
4	P	118/145 (81%)	117 (99%)	1 (1%)	0	100	100
5	Q	120/146 (82%)	116 (97%)	4 (3%)	0	100	100
6	R	120/135 (89%)	115 (96%)	4 (3%)	1 (1%)	16	50
7	S	128/152 (84%)	121 (94%)	7 (6%)	0	100	100
8	T	142/145 (98%)	138 (97%)	4 (3%)	0	100	100
9	Z	70/125 (56%)	66 (94%)	4 (6%)	0	100	100
10	c	59/69 (86%)	57 (97%)	2 (3%)	0	100	100
11	f	71/156 (46%)	64 (90%)	6 (8%)	1 (1%)	9	36
12	A	214/295 (72%)	203 (95%)	11 (5%)	0	100	100
13	B	211/264 (80%)	202 (96%)	9 (4%)	0	100	100
14	C	216/293 (74%)	209 (97%)	6 (3%)	1 (0%)	24	60
15	E	260/263 (99%)	253 (97%)	7 (3%)	0	100	100
16	G	228/249 (92%)	223 (98%)	5 (2%)	0	100	100
17	H	184/194 (95%)	179 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	I	203/208 (98%)	197 (97%)	6 (3%)	0	100	100
19	J	178/194 (92%)	173 (97%)	4 (2%)	1 (1%)	21	56
20	L	149/158 (94%)	144 (97%)	5 (3%)	0	100	100
21	N	147/151 (97%)	146 (99%)	1 (1%)	0	100	100
22	O	133/151 (88%)	125 (94%)	8 (6%)	0	100	100
23	V	80/83 (96%)	78 (98%)	2 (2%)	0	100	100
24	W	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
25	X	139/143 (97%)	134 (96%)	4 (3%)	1 (1%)	18	53
26	Y	122/133 (92%)	119 (98%)	3 (2%)	0	100	100
27	b	80/84 (95%)	77 (96%)	3 (4%)	0	100	100
28	e	53/59 (90%)	50 (94%)	3 (6%)	0	100	100
29	x	176/252 (70%)	172 (98%)	4 (2%)	0	100	100
30	y	319/412 (77%)	303 (95%)	16 (5%)	0	100	100
31	u	619/804 (77%)	592 (96%)	27 (4%)	0	100	100
32	w	247/437 (56%)	241 (98%)	6 (2%)	0	100	100
33	t	119/475 (25%)	103 (87%)	15 (13%)	1 (1%)	16	50
34	K	899/1297 (69%)	858 (95%)	40 (4%)	1 (0%)	48	80
All	All	6239/8138 (77%)	5988 (96%)	244 (4%)	7 (0%)	49	80

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
34	K	379	PRO
11	f	85	TYR
19	J	138	ARG
6	R	67	ARG
14	C	135	GLY
33	t	261	GLU
25	X	86	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	159/170 (94%)	159 (100%)	0	100	100
3	M	104/108 (96%)	104 (100%)	0	100	100
4	P	107/130 (82%)	107 (100%)	0	100	100
5	Q	103/121 (85%)	103 (100%)	0	100	100
6	R	110/122 (90%)	107 (97%)	3 (3%)	39	71
7	S	114/132 (86%)	113 (99%)	1 (1%)	70	85
8	T	114/115 (99%)	114 (100%)	0	100	100
9	Z	64/103 (62%)	64 (100%)	0	100	100
10	c	52/62 (84%)	52 (100%)	0	100	100
11	f	65/140 (46%)	65 (100%)	0	100	100
12	A	180/243 (74%)	180 (100%)	0	100	100
13	B	194/231 (84%)	194 (100%)	0	100	100
14	C	184/225 (82%)	184 (100%)	0	100	100
15	E	224/225 (100%)	224 (100%)	0	100	100
16	G	200/218 (92%)	200 (100%)	0	100	100
17	H	167/174 (96%)	167 (100%)	0	100	100
18	I	178/180 (99%)	178 (100%)	0	100	100
19	J	160/168 (95%)	160 (100%)	0	100	100
20	L	135/142 (95%)	135 (100%)	0	100	100
21	N	130/131 (99%)	130 (100%)	0	100	100
22	O	105/119 (88%)	105 (100%)	0	100	100
23	V	66/67 (98%)	66 (100%)	0	100	100
24	W	112/113 (99%)	112 (100%)	0	100	100
25	X	113/115 (98%)	113 (100%)	0	100	100
26	Y	108/115 (94%)	108 (100%)	0	100	100
27	b	74/76 (97%)	74 (100%)	0	100	100
28	e	45/48 (94%)	45 (100%)	0	100	100
29	x	150/208 (72%)	150 (100%)	0	100	100
30	y	285/367 (78%)	285 (100%)	0	100	100
31	u	550/705 (78%)	550 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	w	217/370 (59%)	217 (100%)	0	100	100
33	t	113/434 (26%)	113 (100%)	0	100	100
34	K	778/1094 (71%)	777 (100%)	1 (0%)	88	93
All	All	5460/6971 (78%)	5455 (100%)	5 (0%)	87	93

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	R	66	VAL
6	R	69	ILE
6	R	78	ARG
7	S	73	ASN
34	K	379	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
2	F	36	GLN
2	F	101	HIS
2	F	137	GLN
7	S	73	ASN
8	T	12	GLN
8	T	105	GLN
12	A	132	GLN
13	B	75	GLN
13	B	202	GLN
14	C	113	GLN
14	C	136	HIS
15	E	138	HIS
15	E	142	HIS
15	E	232	ASN
16	G	4	ASN
16	G	177	GLN
16	G	197	GLN
16	G	202	ASN
16	G	227	GLN
17	H	44	ASN
17	H	97	GLN
18	I	52	ASN
18	I	99	ASN

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Mol	Chain	Res	Type
18	I	155	ASN
18	I	165	GLN
18	I	181	GLN
19	J	75	ASN
19	J	143	ASN
21	N	13	GLN
21	N	36	GLN
21	N	62	GLN
22	O	32	HIS
23	V	33	GLN
28	e	37	GLN
29	x	102	HIS
29	x	216	GLN
30	y	26	ASN
30	y	85	GLN
30	y	92	GLN
30	y	108	GLN
30	y	117	GLN
30	y	124	HIS
30	y	218	GLN
30	y	307	HIS
31	u	101	GLN
31	u	226	GLN
31	u	256	HIS
31	u	286	ASN
31	u	501	GLN
32	w	232	GLN
32	w	397	GLN
33	t	465	ASN
34	K	247	HIS
34	K	290	GLN
34	K	400	ASN
34	K	506	HIS
34	K	549	GLN
34	K	811	GLN
34	K	813	HIS
34	K	1006	ASN
34	K	1034	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1609/1873 (85%)	399 (24%)	23 (1%)

All (399) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	3	C
1	2	9	U
1	2	17	C
1	2	26	U
1	2	33	G
1	2	37	C
1	2	41	G
1	2	42	A
1	2	44	U
1	2	46	A
1	2	56	G
1	2	58	C
1	2	61	A
1	2	62	G
1	2	66	G
1	2	67	C
1	2	68	A
1	2	70	G
1	2	72	C
1	2	73	C
1	2	74	G
1	2	75	G
1	2	76	U
1	2	77	A
1	2	79	A
1	2	92	A
1	2	103	A
1	2	113	G
1	2	114	G
1	2	115	U
1	2	126	G
1	2	127	C
1	2	128	U
1	2	130	G
1	2	143	U
1	2	144	U
1	2	155	G
1	2	163	U

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Mol	Chain	Res	Type
1	2	168	C
1	2	172	U
1	2	181	A
1	2	182	C
1	2	184	G
1	2	215	G
1	2	291	G
1	2	292	A
1	2	295	C
1	2	308	G
1	2	309	G
1	2	310	C
1	2	313	A
1	2	315	C
1	2	318	A
1	2	319	C
1	2	332	G
1	2	333	G
1	2	337	C
1	2	338	G
1	2	347	G
1	2	357	C
1	2	360	A
1	2	362	C
1	2	364	A
1	2	370	G
1	2	377	G
1	2	384	U
1	2	385	G
1	2	386	C
1	2	387	C
1	2	400	C
1	2	407	G
1	2	408	A
1	2	409	C
1	2	413	G
1	2	418	A
1	2	421	G
1	2	437	G
1	2	441	C
1	2	448	A
1	2	450	C

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Mol	Chain	Res	Type
1	2	463	C
1	2	465	A
1	2	466	G
1	2	471	G
1	2	472	C
1	2	473	A
1	2	474	G
1	2	476	A
1	2	482	G
1	2	487	U
1	2	492	C
1	2	502	C
1	2	516	A
1	2	517	C
1	2	525	A
1	2	530	U
1	2	531	A
1	2	537	C
1	2	544	G
1	2	545	A
1	2	548	C
1	2	552	G
1	2	554	A
1	2	555	A
1	2	556	U
1	2	559	G
1	2	560	A
1	2	568	C
1	2	576	A
1	2	583	A
1	2	587	A
1	2	588	G
1	2	589	G
1	2	590	A
1	2	591	U
1	2	594	A
1	2	598	G
1	2	604	A
1	2	605	A
1	2	606	G
1	2	608	C
1	2	614	C

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Mol	Chain	Res	Type
1	2	617	G
1	2	628	A
1	2	629	A
1	2	631	U
1	2	643	A
1	2	644	G
1	2	655	A
1	2	660	C
1	2	664	A
1	2	669	A
1	2	670	A
1	2	671	A
1	2	672	A
1	2	673	G
1	2	685	A
1	2	688	U
1	2	749	U
1	2	750	C
1	2	751	G
1	2	792	C
1	2	794	A
1	2	797	C
1	2	799	U
1	2	809	A
1	2	810	A
1	2	812	A
1	2	821	G
1	2	822	U
1	2	830	A
1	2	844	U
1	2	847	A
1	2	852	G
1	2	853	C
1	2	856	C
1	2	869	A
1	2	870	A
1	2	871	U
1	2	872	A
1	2	873	G
1	2	874	G
1	2	878	G
1	2	880	G

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Mol	Chain	Res	Type
1	2	885	U
1	2	886	A
1	2	887	U
1	2	888	U
1	2	889	U
1	2	890	U
1	2	891	G
1	2	892	U
1	2	893	U
1	2	895	G
1	2	896	U
1	2	898	U
1	2	903	A
1	2	905	C
1	2	907	G
1	2	908	A
1	2	913	A
1	2	914	U
1	2	918	U
1	2	919	A
1	2	920	A
1	2	933	G
1	2	943	U
1	2	959	G
1	2	963	A
1	2	970	G
1	2	971	G
1	2	978	G
1	2	981	A
1	2	990	A
1	2	992	A
1	2	1001	A
1	2	1002	U
1	2	1008	A
1	2	1009	A
1	2	1017	U
1	2	1023	A
1	2	1027	A
1	2	1028	A
1	2	1031	A
1	2	1040	G
1	2	1041	G

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Mol	Chain	Res	Type
1	2	1049	A
1	2	1057	C
1	2	1058	A
1	2	1059	G
1	2	1078	C
1	2	1080	A
1	2	1083	A
1	2	1085	C
1	2	1086	G
1	2	1087	A
1	2	1088	U
1	2	1096	G
1	2	1100	A
1	2	1109	C
1	2	1114	U
1	2	1116	C
1	2	1117	C
1	2	1118	C
1	2	1119	A
1	2	1126	G
1	2	1133	A
1	2	1138	C
1	2	1143	A
1	2	1148	A
1	2	1153	C
1	2	1154	U
1	2	1155	U
1	2	1157	G
1	2	1171	G
1	2	1195	A
1	2	1200	A
1	2	1204	A
1	2	1205	C
1	2	1207	G
1	2	1208	A
1	2	1211	G
1	2	1215	C
1	2	1217	A
1	2	1221	G
1	2	1224	G
1	2	1227	G
1	2	1232	U

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Mol	Chain	Res	Type
1	2	1240	A
1	2	1242	U
1	2	1243	U
1	2	1248	U
1	2	1249	C
1	2	1250	A
1	2	1251	A
1	2	1254	C
1	2	1255	G
1	2	1256	G
1	2	1257	G
1	2	1258	A
1	2	1259	A
1	2	1260	A
1	2	1261	C
1	2	1264	C
1	2	1265	A
1	2	1273	C
1	2	1274	G
1	2	1284	A
1	2	1285	G
1	2	1286	G
1	2	1297	U
1	2	1298	G
1	2	1299	A
1	2	1300	U
1	2	1301	A
1	2	1302	G
1	2	1304	U
1	2	1305	C
1	2	1306	U
1	2	1308	U
1	2	1309	C
1	2	1313	A
1	2	1315	U
1	2	1316	C
1	2	1317	C
1	2	1321	G
1	2	1322	G
1	2	1323	U
1	2	1324	G
1	2	1325	G

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Mol	Chain	Res	Type
1	2	1335	G
1	2	1338	G
1	2	1339	U
1	2	1348	G
1	2	1358	U
1	2	1372	U
1	2	1378	A
1	2	1382	A
1	2	1388	A
1	2	1389	C
1	2	1396	A
1	2	1397	U
1	2	1398	G
1	2	1445	U
1	2	1446	A
1	2	1454	A
1	2	1455	A
1	2	1462	U
1	2	1463	U
1	2	1464	C
1	2	1465	A
1	2	1466	G
1	2	1476	A
1	2	1477	U
1	2	1489	A
1	2	1490	G
1	2	1491	G
1	2	1492	U
1	2	1494	U
1	2	1495	G
1	2	1497	G
1	2	1498	A
1	2	1505	U
1	2	1506	A
1	2	1507	G
1	2	1509	U
1	2	1512	C
1	2	1519	U
1	2	1526	G
1	2	1531	A
1	2	1533	A
1	2	1534	C

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Mol	Chain	Res	Type
1	2	1535	U
1	2	1544	C
1	2	1548	G
1	2	1551	U
1	2	1559	C
1	2	1560	U
1	2	1566	G
1	2	1567	G
1	2	1571	G
1	2	1574	C
1	2	1575	G
1	2	1579	A
1	2	1580	A
1	2	1581	C
1	2	1582	C
1	2	1584	G
1	2	1585	U
1	2	1586	U
1	2	1587	G
1	2	1600	G
1	2	1601	A
1	2	1602	U
1	2	1606	G
1	2	1612	G
1	2	1617	G
1	2	1618	C
1	2	1621	U
1	2	1623	A
1	2	1628	C
1	2	1632	G
1	2	1647	A
1	2	1648	G
1	2	1649	U
1	2	1654	G
1	2	1663	A
1	2	1665	G
1	2	1671	G
1	2	1675	A
1	2	1686	G
1	2	1699	A
1	2	1714	U
1	2	1721	U

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Mol	Chain	Res	Type
1	2	1722	G
1	2	1723	G
1	2	1727	G
1	2	1729	U
1	2	1744	G
1	2	1751	C
1	2	1756	C
1	2	1776	G
1	2	1783	C
1	2	1784	G
1	2	1786	U
1	2	1801	A
1	2	1808	U
1	2	1816	G
1	2	1819	A
1	2	1826	G
1	2	1844	U
1	2	1859	A
1	2	1861	G
1	2	1863	A
1	2	1864	U
1	2	1870	A
1	2	1871	C
1	2	1872	G
1	2	1873	G

All (23) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	102	A
1	2	114	G
1	2	143	U
1	2	180	G
1	2	291	G
1	2	314	U
1	2	332	G
1	2	465	A
1	2	547	G
1	2	604	A
1	2	811	A
1	2	958	G
1	2	980	A

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Mol	Chain	Res	Type
1	2	1231	C
1	2	1316	C
1	2	1338	G
1	2	1493	C
1	2	1511	U
1	2	1534	C
1	2	1558	C
1	2	1601	A
1	2	1648	G
1	2	1726	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

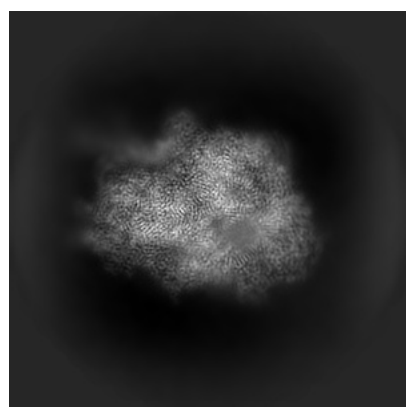
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32806. These allow visual inspection of the internal detail of the map and identification of artifacts.

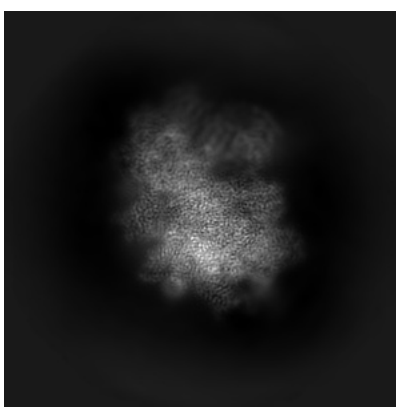
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

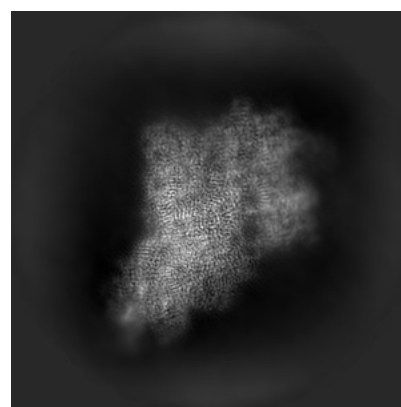
6.1.1 Primary map



X



Y

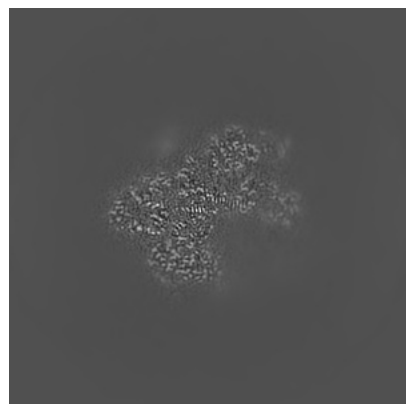


Z

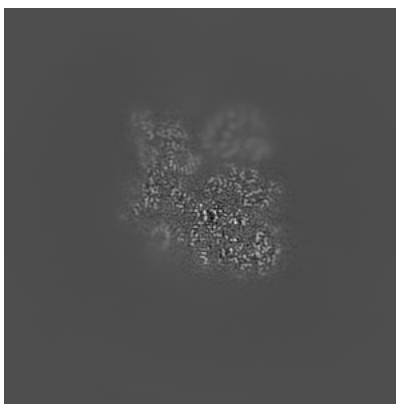
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

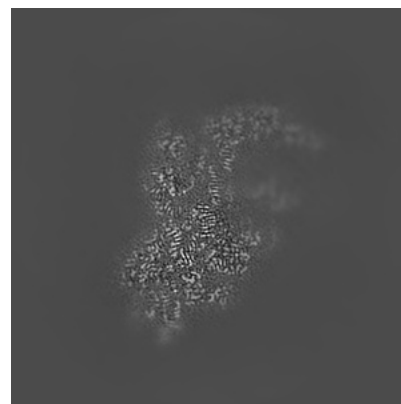
6.2.1 Primary map



X Index: 180



Y Index: 180

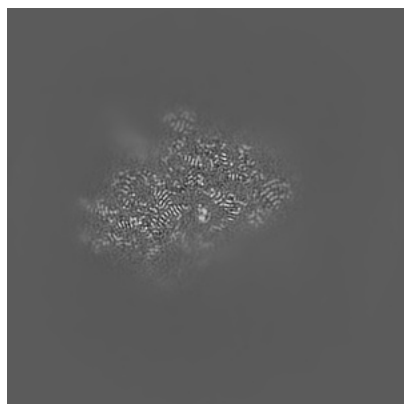


Z Index: 180

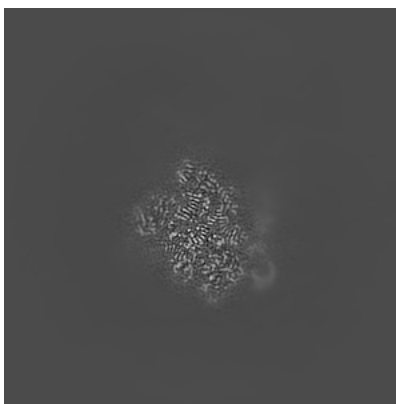
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

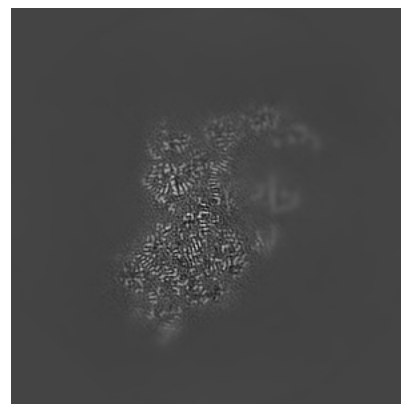
6.3.1 Primary map



X Index: 148



Y Index: 133

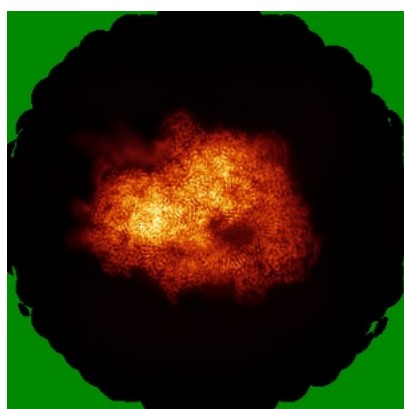


Z Index: 183

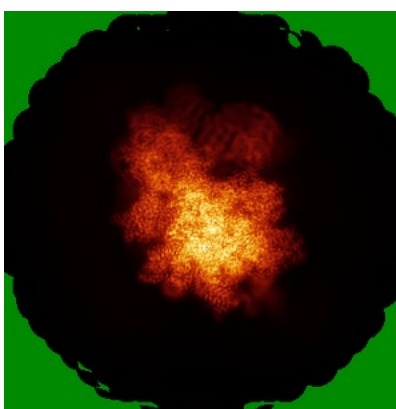
The images above show the largest variance slices of the map in three orthogonal directions.

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

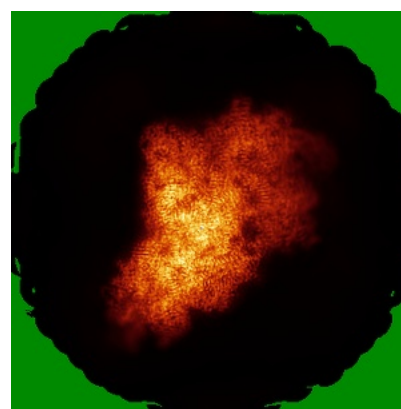
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

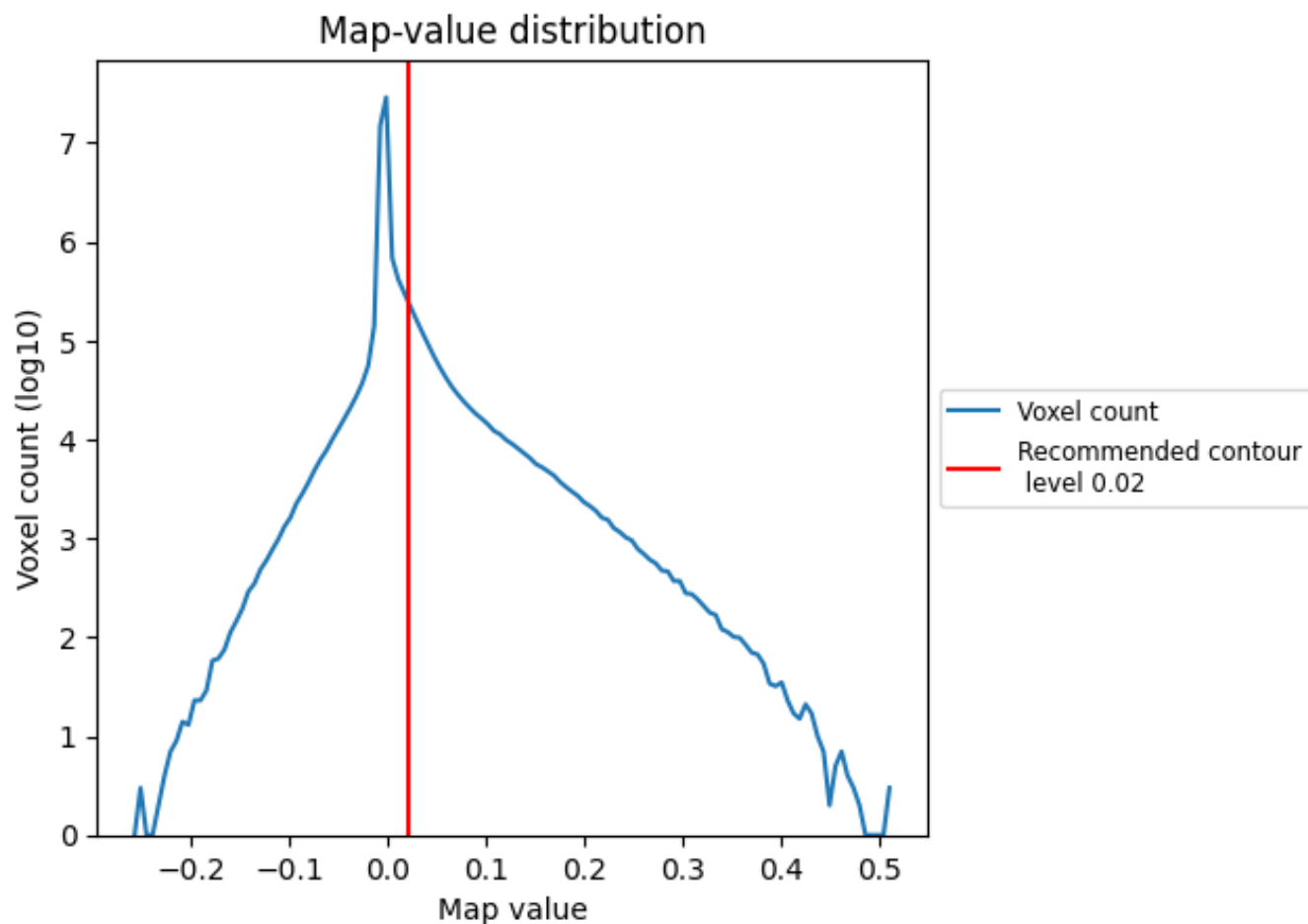
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

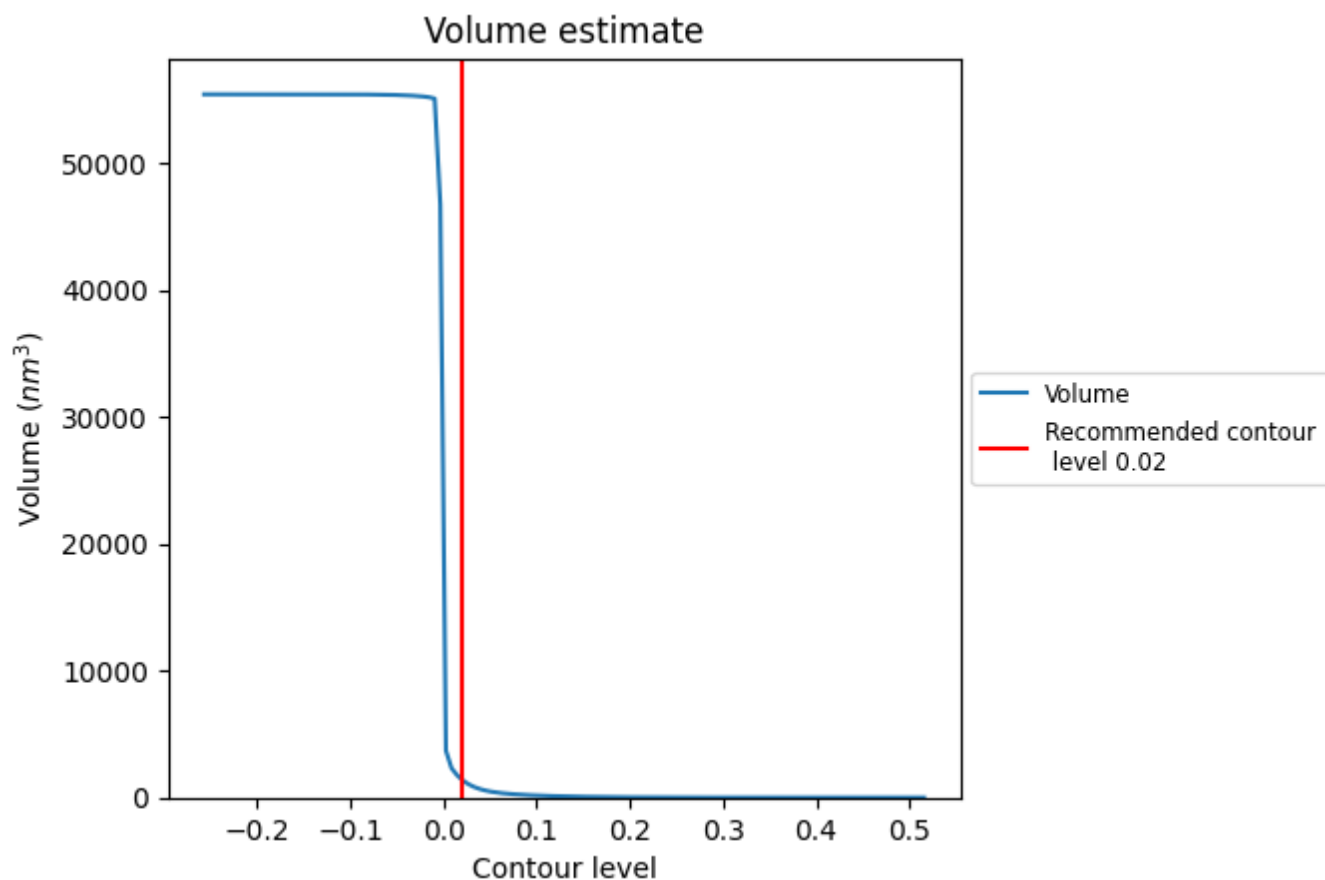
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

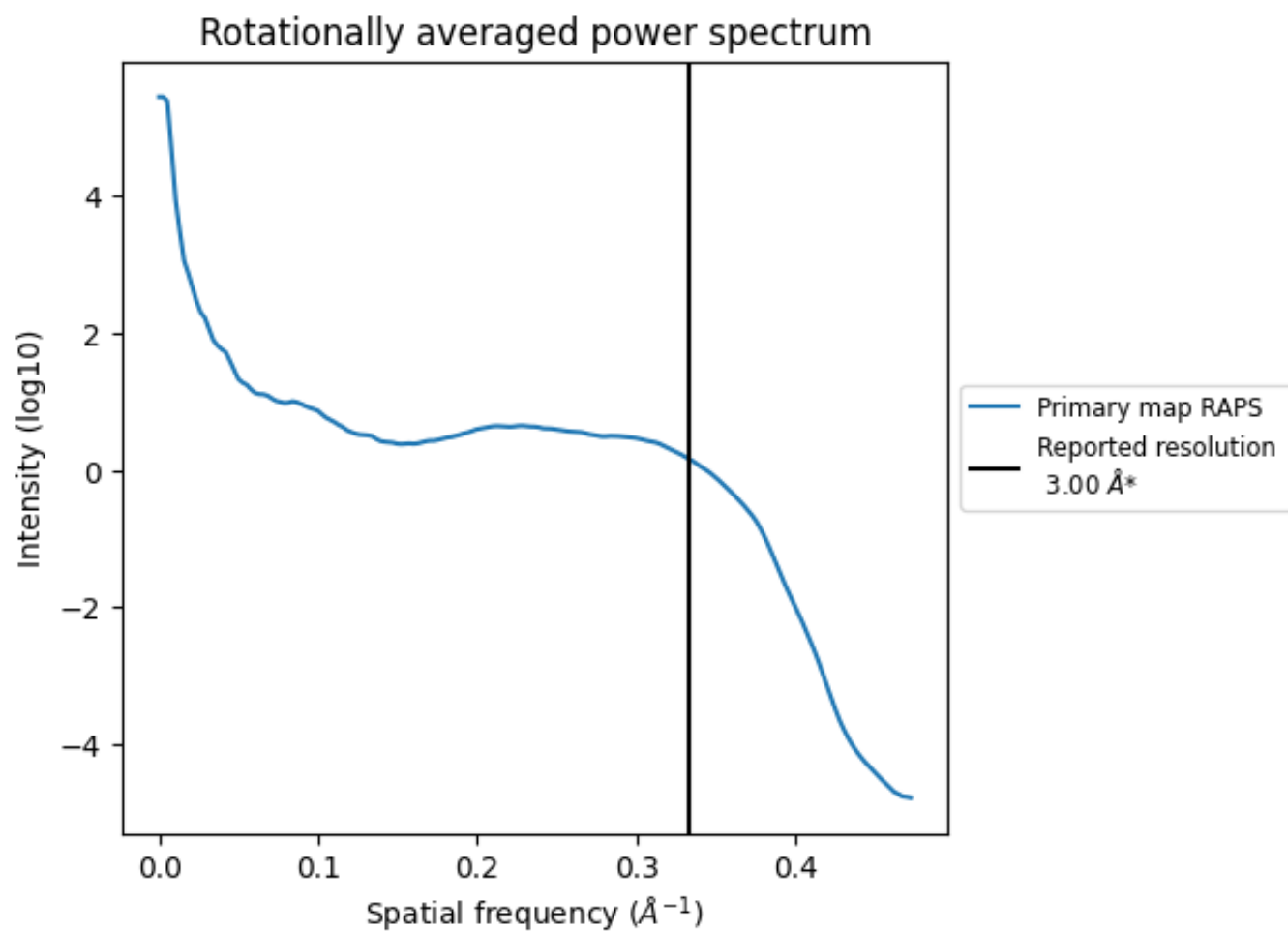
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1392 nm^3 ; this corresponds to an approximate mass of 1257 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 ⓘ

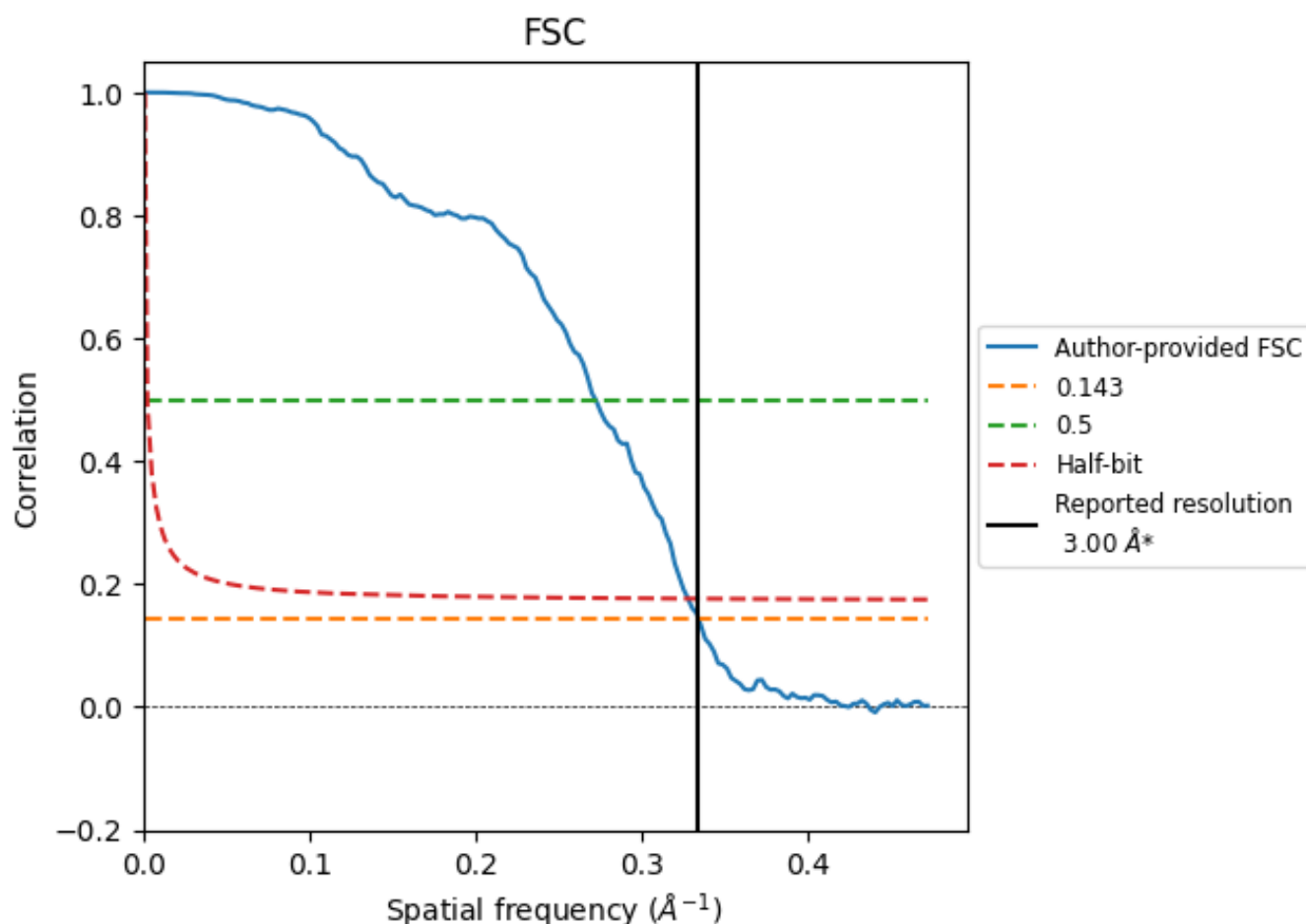


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

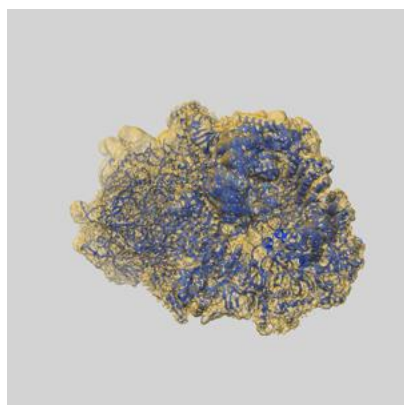
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.99	3.67	3.05
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

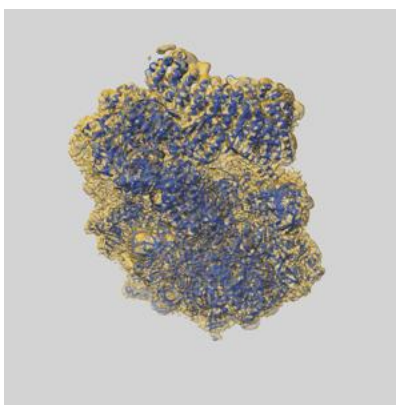
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32806 and PDB model 7WTZ. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

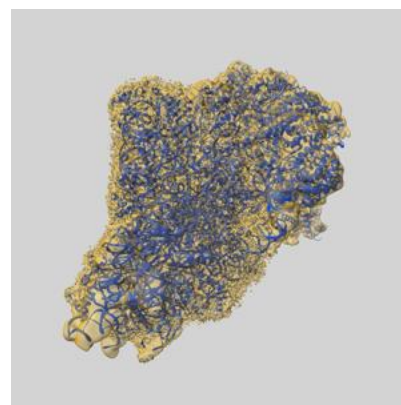
9.1 Map-model overlay [i](#)



X



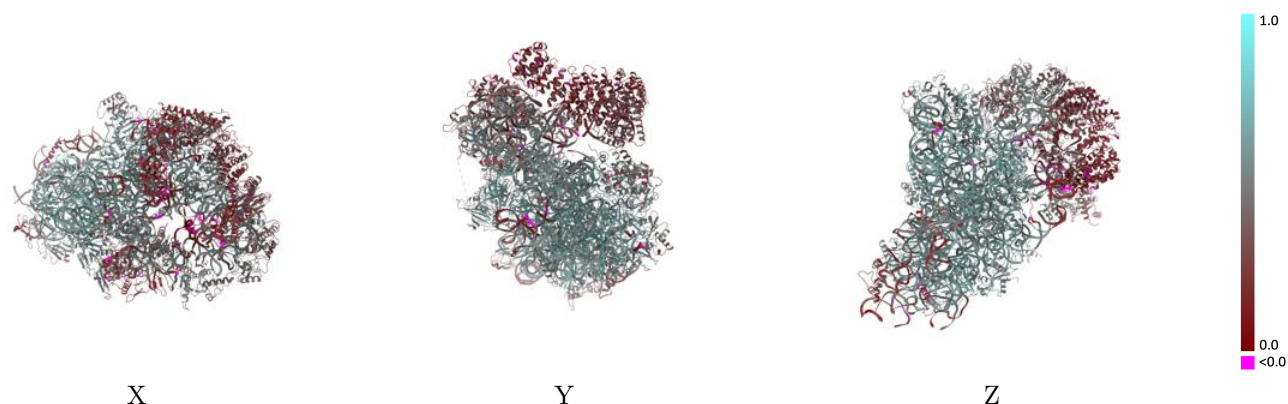
Y



Z

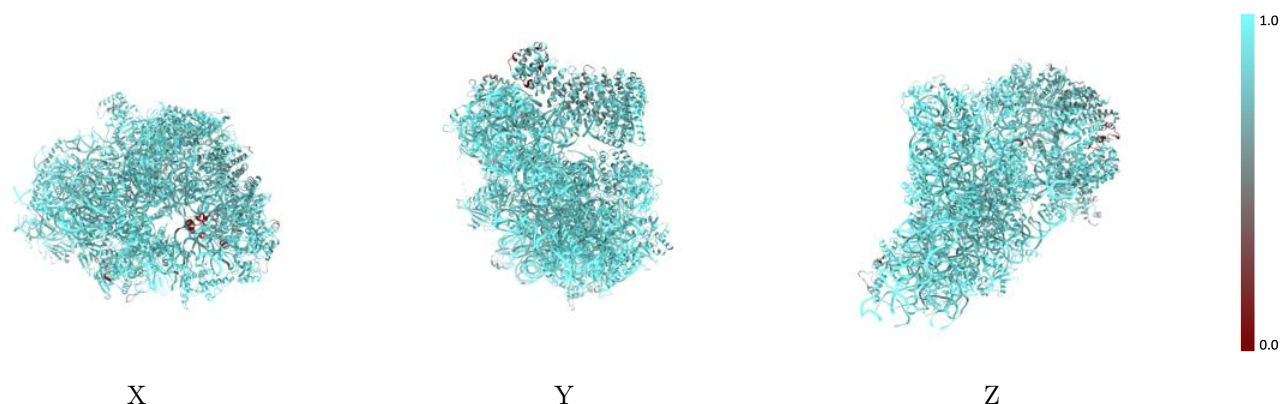
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



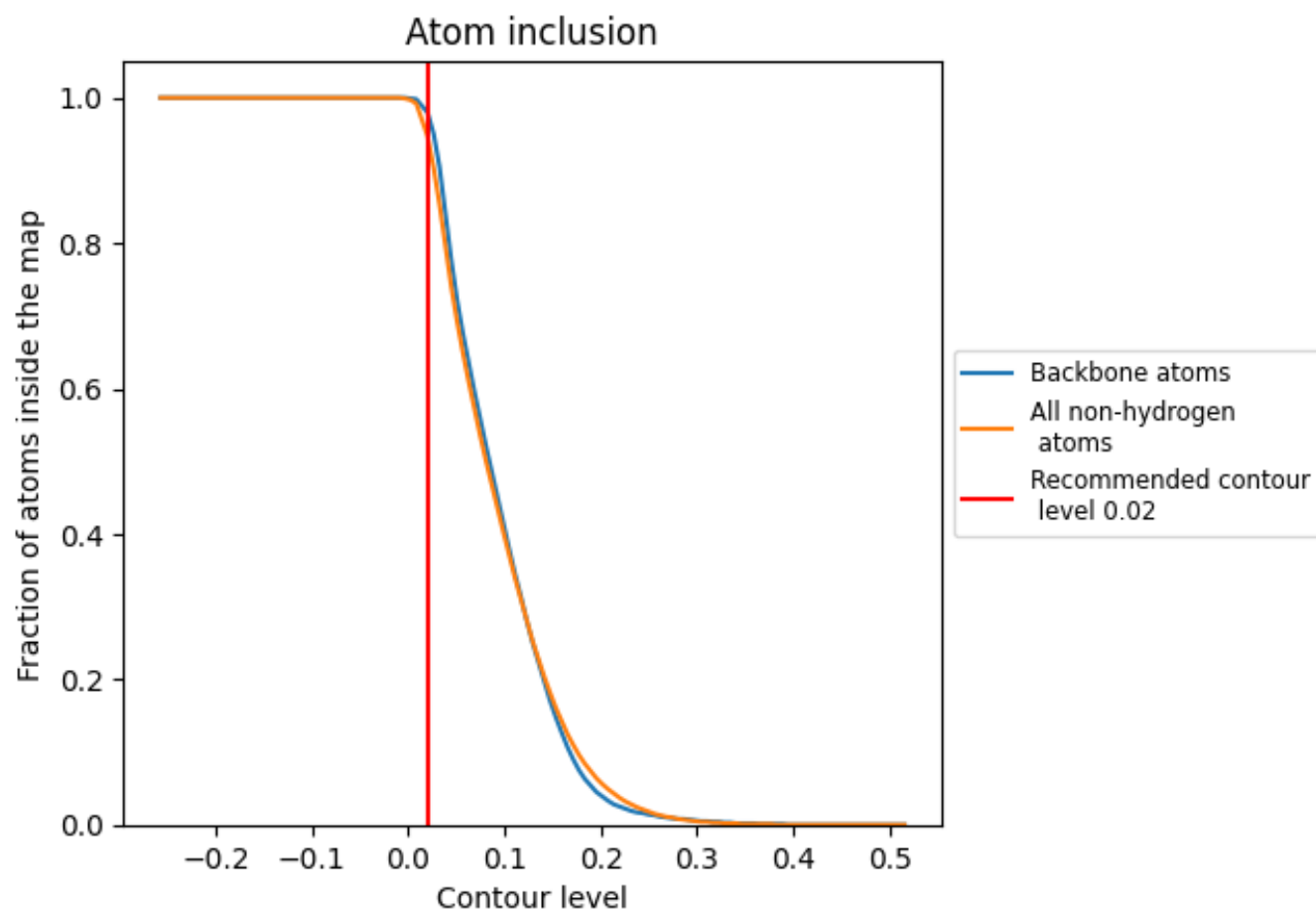
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion ⓘ



At the recommended contour level, 98% of all backbone atoms, 95% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9480	 0.4820
2	 0.9800	 0.5120
A	 0.9840	 0.5950
B	 0.9720	 0.5500
C	 0.9760	 0.5750
E	 0.9880	 0.5990
F	 0.9590	 0.4690
G	 0.8940	 0.3840
H	 0.9190	 0.4580
I	 0.9320	 0.4990
J	 0.9820	 0.5940
K	 0.7770	 0.2080
L	 0.9590	 0.5620
M	 0.7610	 0.2530
N	 0.9950	 0.5720
O	 0.9620	 0.5170
P	 0.9560	 0.4960
Q	 0.8930	 0.4060
R	 0.9010	 0.3720
S	 0.9150	 0.4220
T	 0.9100	 0.4370
V	 0.9800	 0.5840
W	 0.9870	 0.6210
X	 0.9890	 0.6190
Y	 0.9920	 0.5720
Z	 0.8540	 0.3730
b	 0.9830	 0.5530
c	 0.9580	 0.4670
e	 0.9200	 0.5180
f	 0.8760	 0.2990
t	 0.9440	 0.4080
u	 0.9720	 0.5370
w	 0.9520	 0.4530
x	 0.9830	 0.5710
y	 0.9410	 0.4470

