



Full wwPDB EM Validation Report ⓘ

Sep 21, 2026 – 11:14 AM EDT

PDB ID : 9YDB / pdb_00009ydb
EMDB ID : EMD-72799
Title : Eukaryotic pre-60S ribosomes from uL16 P-site loop mutants in bypass condition. Lsg1,Nmd3 and Tif6 present
Authors : Guan, K.; Taylor, D.W.
Deposited on : 2025-09-22
Resolution : 2.83 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:

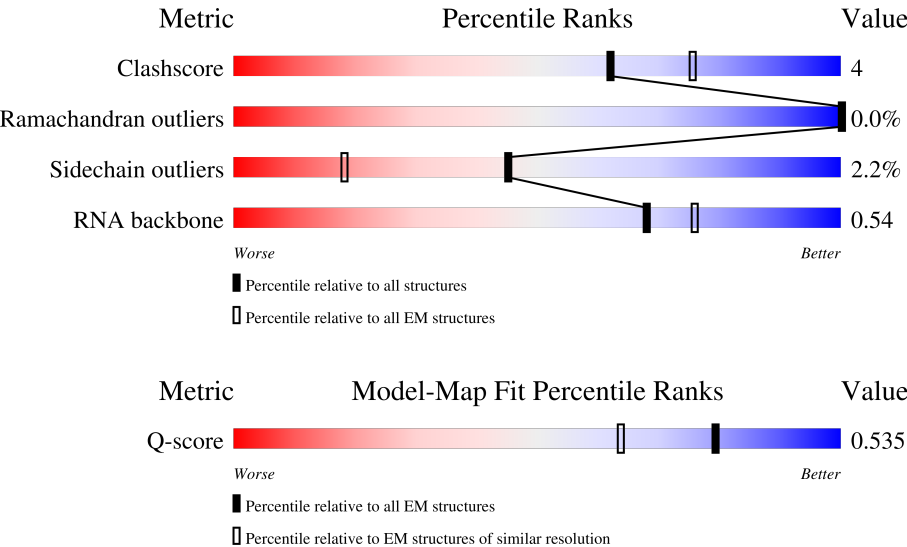
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

1 Overall quality at a glance

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

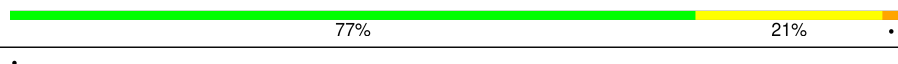
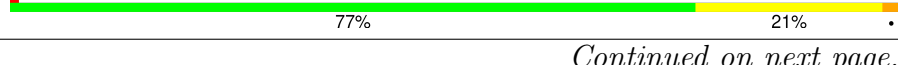
The reported resolution of this entry is 2.83 Å.

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.



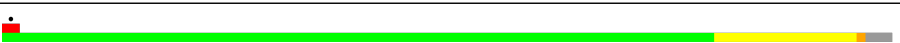
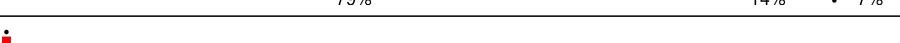
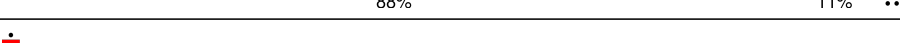
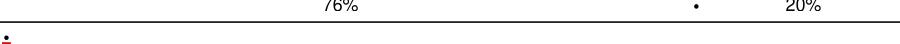
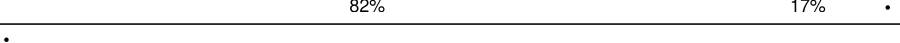
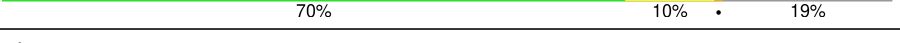
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11847 (2.33 - 3.33)

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

Mol	Chain	Length	Quality of chain
1	A	3396	
2	B	121	
3	C	158	

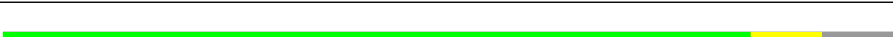
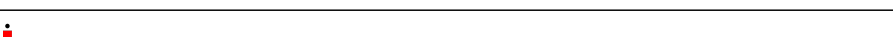
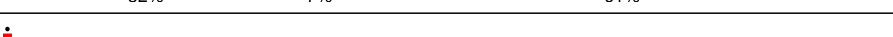
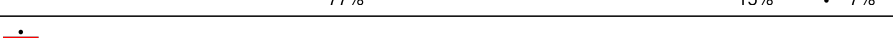
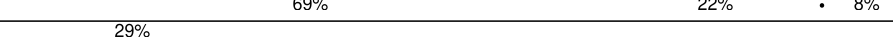
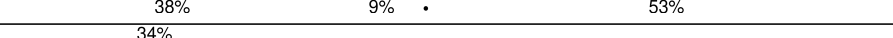
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Mol	Chain	Length	Quality of chain
4	z	432	
5	LD	254	
6	LE	387	
7	LF	362	
8	LG	297	
9	LH	176	
10	LI	244	
11	LJ	256	
12	LK	191	
13	LL	210	
14	LM	174	
15	LN	199	
16	LO	138	
17	LP	204	
18	LQ	199	
19	LR	184	
20	LS	186	
21	LT	189	
22	LU	172	
23	LV	160	
24	LW	121	
25	LX	137	
26	LY	155	
27	LZ	142	
28	La	127	

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Mol	Chain	Length	Quality of chain
29	Lb	136	
30	Lc	149	
31	Ld	59	
32	Le	105	
33	Lf	113	
34	Lg	130	
35	Lh	107	
36	Li	121	
37	Lj	120	
38	Lk	100	
39	Ll	88	
40	Lm	78	
41	Ln	51	
42	Lo	128	
43	Lq	106	
44	Lr	92	
45	X	245	
46	W	640	
47	V	518	

2 Entry composition [i](#)

There are 48 unique types of molecules in this entry. The entry contains 126907 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 25S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3023	Total	C	N	O	P	0	0
			64684	28892	11687	21082	3023		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	493	U	G	conflict	GB 831416132

- Molecule 2 is a RNA chain called 5S RNA.

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

- Molecule 3 is a RNA chain called 8S RNA.

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

- Molecule 4 is a protein called Cytoplasmic 60S subunit biogenesis factor REH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	z	56	Total	C	N	O	S	0	0
			469	289	92	85	3		

- Molecule 5 is a protein called 60S ribosomal protein L2-A.

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

- Molecule 6 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	LE	386	Total	C	N	O	S	0	0
			3081	1956	584	533	8		

- Molecule 7 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	LF	361	Total	C	N	O	S	0	0
			2749	1730	522	494	3		

- Molecule 8 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LG	286	Total	C	N	O	S	0	0
			2298	1453	400	443	2		

- Molecule 9 is a protein called Large ribosomal subunit protein eL6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LH	156	Total	C	N	O		0	0
			1243	803	222	218			

- Molecule 10 is a protein called 60S ribosomal protein L7-A.

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

- Molecule 11 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LJ	228	Total	C	N	O	S	0	0
			1780	1137	318	322	3		

- Molecule 12 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LK	188	Total	C	N	O	S	0	0
			1493	948	271	270	4		

- Molecule 13 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LL	207	Total	C	N	O	S	0	0
			1686	1071	319	291	5		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LL	?	-	MET	deletion	UNP P41805
LL	?	-	LEU	deletion	UNP P41805
LL	?	-	SER	deletion	UNP P41805
LL	?	-	CYS	deletion	UNP P41805
LL	?	-	ALA	deletion	UNP P41805
LL	?	-	GLY	deletion	UNP P41805
LL	?	-	ALA	deletion	UNP P41805
LL	?	-	ASP	deletion	UNP P41805
LL	?	-	ARG	deletion	UNP P41805
LL	?	-	LEU	deletion	UNP P41805
LL	?	-	GLN	deletion	UNP P41805

- Molecule 14 is a protein called Large ribosomal subunit protein uL5B.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LM	167	Total	C	N	O	S	0	0
			1336	838	249	245	4		

- Molecule 15 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LN	193	Total	C	N	O		0	0
			1543	962	315	266			

- Molecule 16 is a protein called 60S ribosomal protein L14-A.

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

- Molecule 17 is a protein called 60S ribosomal protein L15-A.

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

- Molecule 18 is a protein called 60S ribosomal protein L16-A.

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

- Molecule 19 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LR	172	Total	C	N	O		0	0
			1361	846	273	242			

- Molecule 20 is a protein called 60S ribosomal protein L18-A.

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

- Molecule 21 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LT	152	Total	C	N	O		0	0
			1228	763	260	205			

- Molecule 22 is a protein called 60S ribosomal protein L20-A.

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

- Molecule 23 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LV	159	Total	C	N	O	S	0	0
			1276	805	246	221	4		

- Molecule 24 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LW	98	Total	C	N	O		0	0
			778	505	127	146			

- Molecule 25 is a protein called 60S ribosomal protein L23-A.

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

- Molecule 26 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LY	62	Total	C	N	O	S	0	0
			513	330	101	81	1		

- Molecule 27 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LZ	120	Total	C	N	O	S	0	0
			959	617	168	172	2		

- Molecule 28 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	La	125	Total	C	N	O		0	0
			984	620	191	173			

- Molecule 29 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Lb	134	Total	C	N	O		0	0
			1087	707	201	179			

- Molecule 30 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Lc	148	Total	C	N	O	S	0	0
			1173	749	231	190	3		

- Molecule 31 is a protein called 60S ribosomal protein L29.

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

- Molecule 32 is a protein called 60S ribosomal protein L30.

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

- Molecule 33 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Lf	105	Total	C	N	O	S	0	0
			856	544	163	148	1		

- Molecule 34 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Lg	126	Total	C	N	O	S	0	0
			1012	641	204	166	1		

- Molecule 35 is a protein called 60S ribosomal protein L33-A.

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

- Molecule 36 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Li	109	Total	C	N	O	S	0	0
			861	533	175	149	4		

- Molecule 37 is a protein called 60S ribosomal protein L35-A.

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

- Molecule 38 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Lk	97	Total	C	N	O	S	0	0
			750	469	149	130	2		

- Molecule 39 is a protein called 60S ribosomal protein L37-A.

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

- Molecule 40 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Lm	76	Total	C	N	O		0	0
			604	385	114	105			

- Molecule 41 is a protein called 60S ribosomal protein L39.

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

- Molecule 42 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Lo	50	Total	C	N	O	S	0	0
			401	247	84	65	5		

- Molecule 43 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Lq	99	Total	C	N	O	S	0	0
			801	504	162	130	5		

- Molecule 44 is a protein called 60S ribosomal protein L43-A.

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

- Molecule 45 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	X	226	Total	C	N	O	S	0	0
			1713	1064	296	346	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	192	PHE	VAL	conflict	UNP Q12522

- Molecule 46 is a protein called Large subunit GTPase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	W	301	Total	C	N	O	S	0	0
			2417	1562	421	429	5		

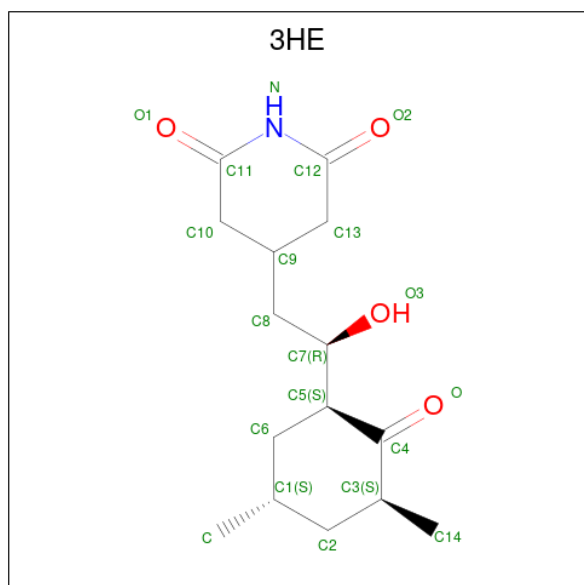
- Molecule 47 is a protein called 60S ribosomal export protein NMD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	V	398	Total	C	N	O	S	0	0
			3159	2016	541	587	15		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	379	ASP	TYR	conflict	UNP P38861

- Molecule 48 is 4-{(2R)-2-[(1S,3S,5S)-3,5-dimethyl-2-oxocyclohexyl]-2-hydroxyethyl}piperidine-2,6-dione (CCD ID: 3HE) (formula: C₁₅H₂₃NO₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
48	A	1	Total	C	N	O	0
			20	15	1	4	



LYS
LEU
SER
GLN
VAL
TYR
GLY
ALA
LYS
ASN
ASP
GLU
GLY
ASP
GLY
VAL
ASP
TLE
THR
VAL
SER
SER
ASN
ASP
TLE
ALA
ASN
TYR
THR
THR
VAL
SER
TLE
ASP
GLU
SER
GLY
LEU
GLU
LEU
THR
THR
PRO
THR
GLY
ALA
ARG
LEU
GLY
HIS
ARG
ALA
GLY
GLN
ARG
TYR

TYR
ARG
GLN
ASN
LEU
PRO
SER
GLN
PRO
ASN
ASN
GLU
SER
ARG
T377
A380
A381
R384
M385
G397
R398
M401
Q402
R414
R415
E416
V420
M421
L431
Q432

• Molecule 5: 60S ribosomal protein L2-A

Chain LD:  77% 20%

MET
G2
N7
R21
L29
D33
R37
K46
T48
V49
H60
D51
R54
G55
A56
K60
R70
I75
H83
Q86
K92
K93
V101
L104
P108
T111
I112
V113
E117
L126
V134
I135
I136
D142
E143
V148
R149

L150
P151
K155
I158
A162
V165
K188
Y189
R190
L191
T199
R200
V207
V230
I238
R242
T243
L245
L246
R247
GLY
SER
GLN
LYS
THR
ASP

• Molecule 6: 60S ribosomal protein L3

Chain LE:  84% 14%

MET
S2
P9
L17
R21
V41
A42
L43
T44
L47
M53
L60
D61
R62
E74
T77
P82
T82
V83
G91
Y92
T96
S297
F298
D299
R300
N319
M323
V324
K325
R332
I335
T346
S347
R348
R349
A350
K357
R369
T372
P373
A374
I381

Q182
G185
I188
V192
M214
V229
V233
K241
T242
H243
V249
A250
H259
Y272
I278
N279
Y283
R284
T296
S297
F298
D299
R300
N319
M323
V324
K325
R332
I335
T346
S347
R348
R349
A350
K357
R369
T372
P373
A374
I381

D386
L387

• Molecule 7: 60S ribosomal protein L4-A

Chain LF:  89% 11%

MET
S2
V8
L11
T16
V35
E54
G57
T60
R84
R98
T129
L136
V142
E143
K144
I145
V151
T154
D155
L156
E157
K170
H175
R188
G192
K193
Y194
P205
V208
V225
A228
L233
L238
L244

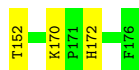
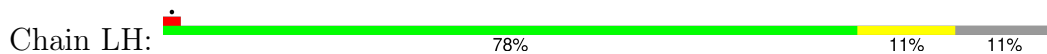
V248
I281
V286
Q304
P317
V323
R326
K346
K350
P351
D362

• Molecule 8: 60S ribosomal protein L5

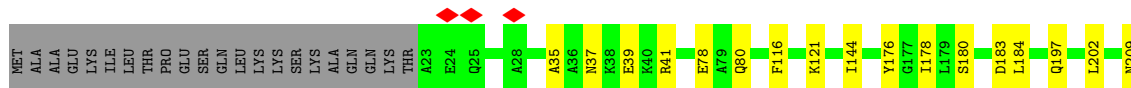
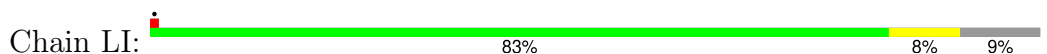
Chain LG:  82% 14%

MET
ALA
PHE
GLN
LYS
ASP
A7
R22
R23
R24
E25
G26
K27
Y30
R33
K41
R54
P84
W95
L103
L104
I105
A106
R107
R108
T109
K112
V122
E123
E124
T132
D137
L146
Q151
G156
V159
L163
G170
M178
P181

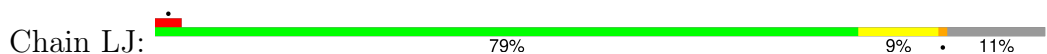
- Molecule 9: Large ribosomal subunit protein eL6B



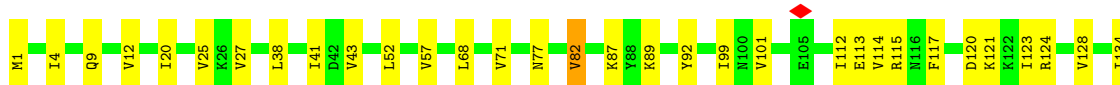
- Molecule 10: 60S ribosomal protein L7-A



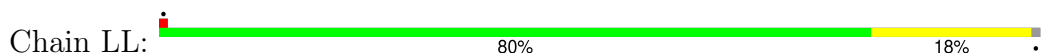
- Molecule 11: 60S ribosomal protein L8-A

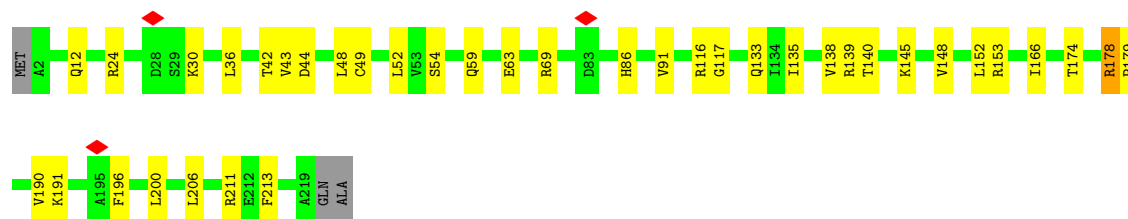


- Molecule 12: 60S ribosomal protein L9-A

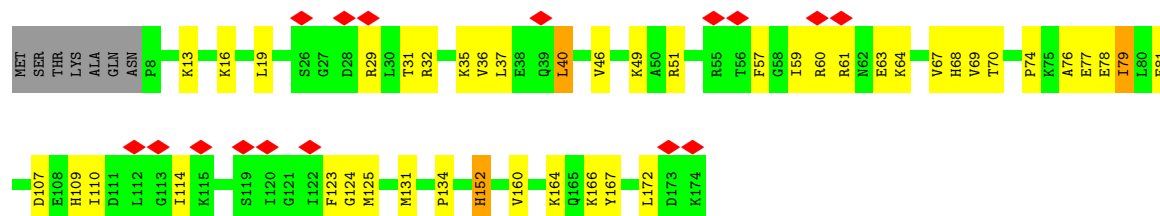


- Molecule 13: Large ribosomal subunit protein uL16

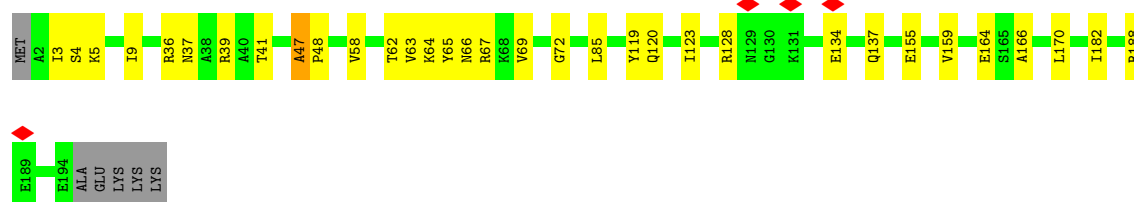
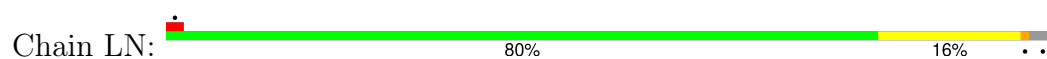




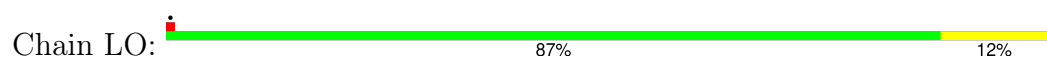
- Molecule 14: Large ribosomal subunit protein uL5B



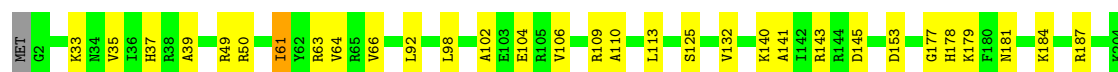
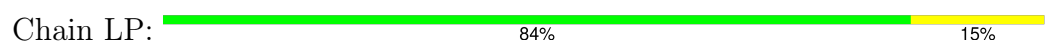
- Molecule 15: 60S ribosomal protein L13-A



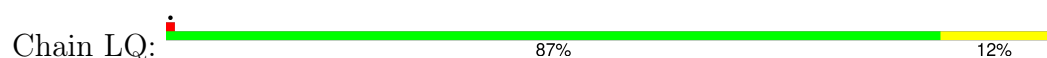
- Molecule 16: 60S ribosomal protein L14-A



- Molecule 17: 60S ribosomal protein L15-A



- Molecule 18: 60S ribosomal protein L16-A





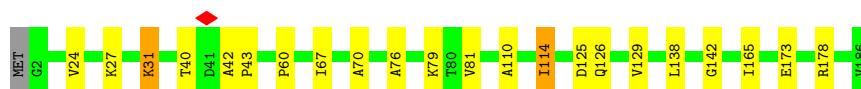
- Molecule 19: 60S ribosomal protein L17-A

Chain LR: 79% 14% 7%



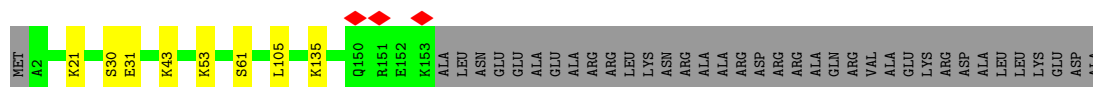
- Molecule 20: 60S ribosomal protein L18-A

Chain LS: 88% 11% ..



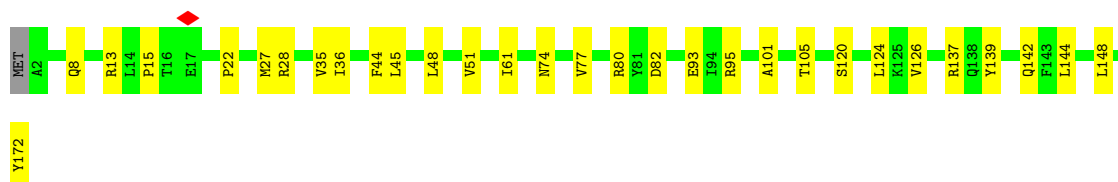
- Molecule 21: 60S ribosomal protein L19-A

Chain LT: 76% 20%



- Molecule 22: 60S ribosomal protein L20-A

Chain LU: 82% 17%



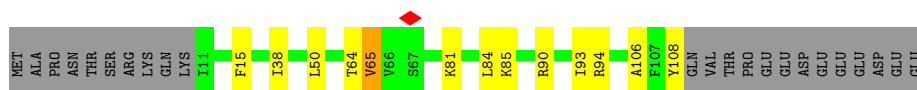
- Molecule 23: 60S ribosomal protein L21-A

Chain LV: 85% 14% ..

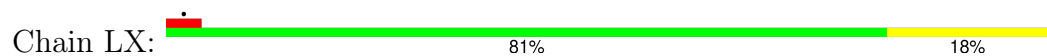


- Molecule 24: 60S ribosomal protein L22-A

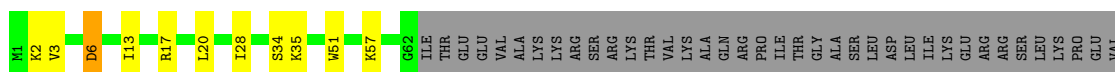
Chain LW: 70% 10% 19%



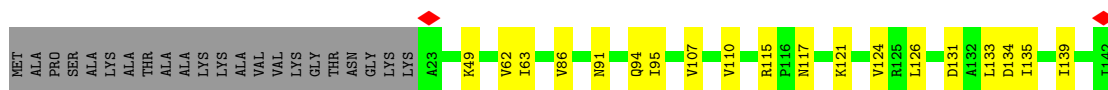
- Molecule 25: 60S ribosomal protein L23-A



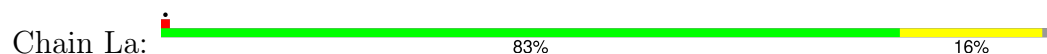
- Molecule 26: 60S ribosomal protein L24-A



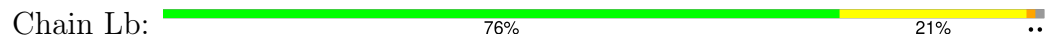
- Molecule 27: 60S ribosomal protein L25



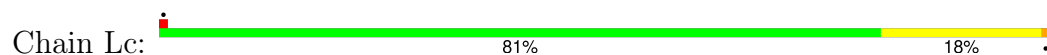
- Molecule 28: 60S ribosomal protein L26-A



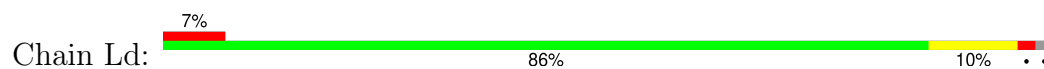
- Molecule 29: 60S ribosomal protein L27-A



- Molecule 30: 60S ribosomal protein L28



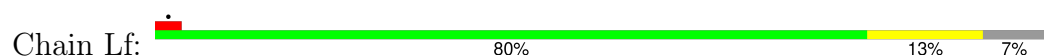
• Molecule 31: 60S ribosomal protein L29



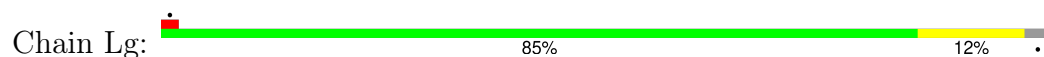
• Molecule 32: 60S ribosomal protein L30



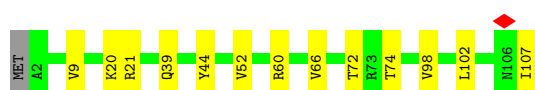
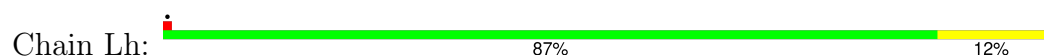
• Molecule 33: 60S ribosomal protein L31-A



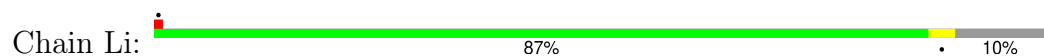
• Molecule 34: 60S ribosomal protein L32



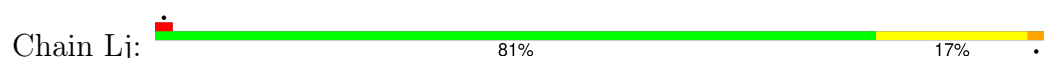
• Molecule 35: 60S ribosomal protein L33-A

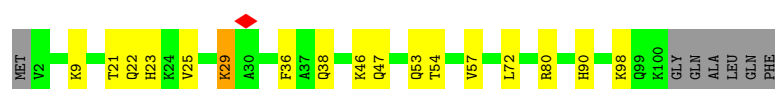


• Molecule 36: 60S ribosomal protein L34-A

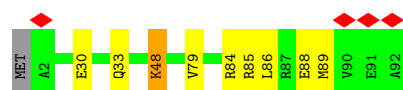


• Molecule 37: 60S ribosomal protein L35-A

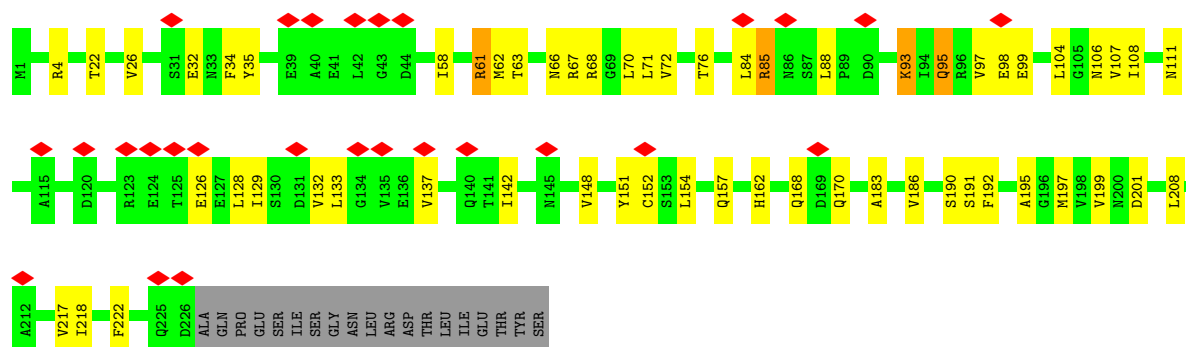




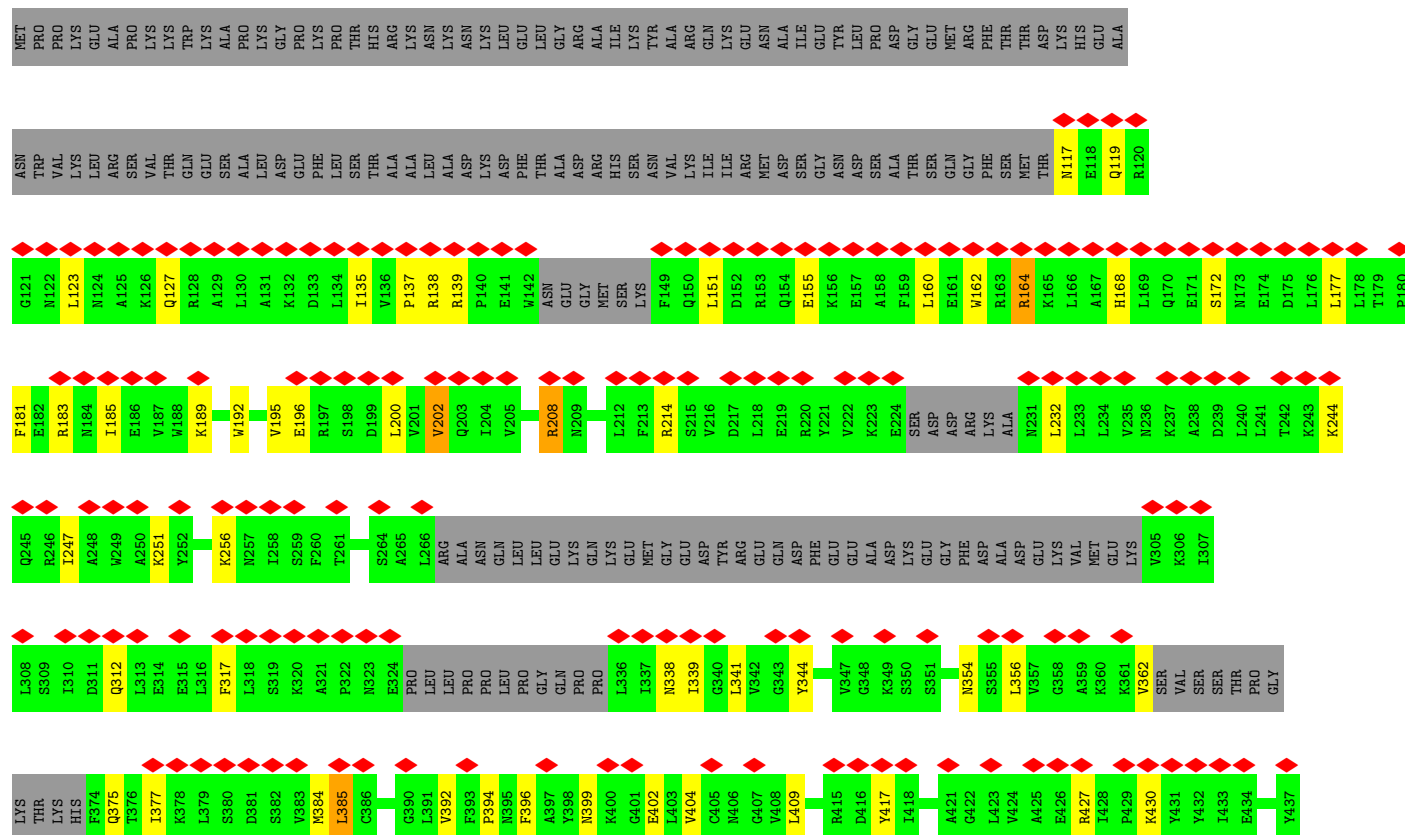
Chain Lr: 89% 9%



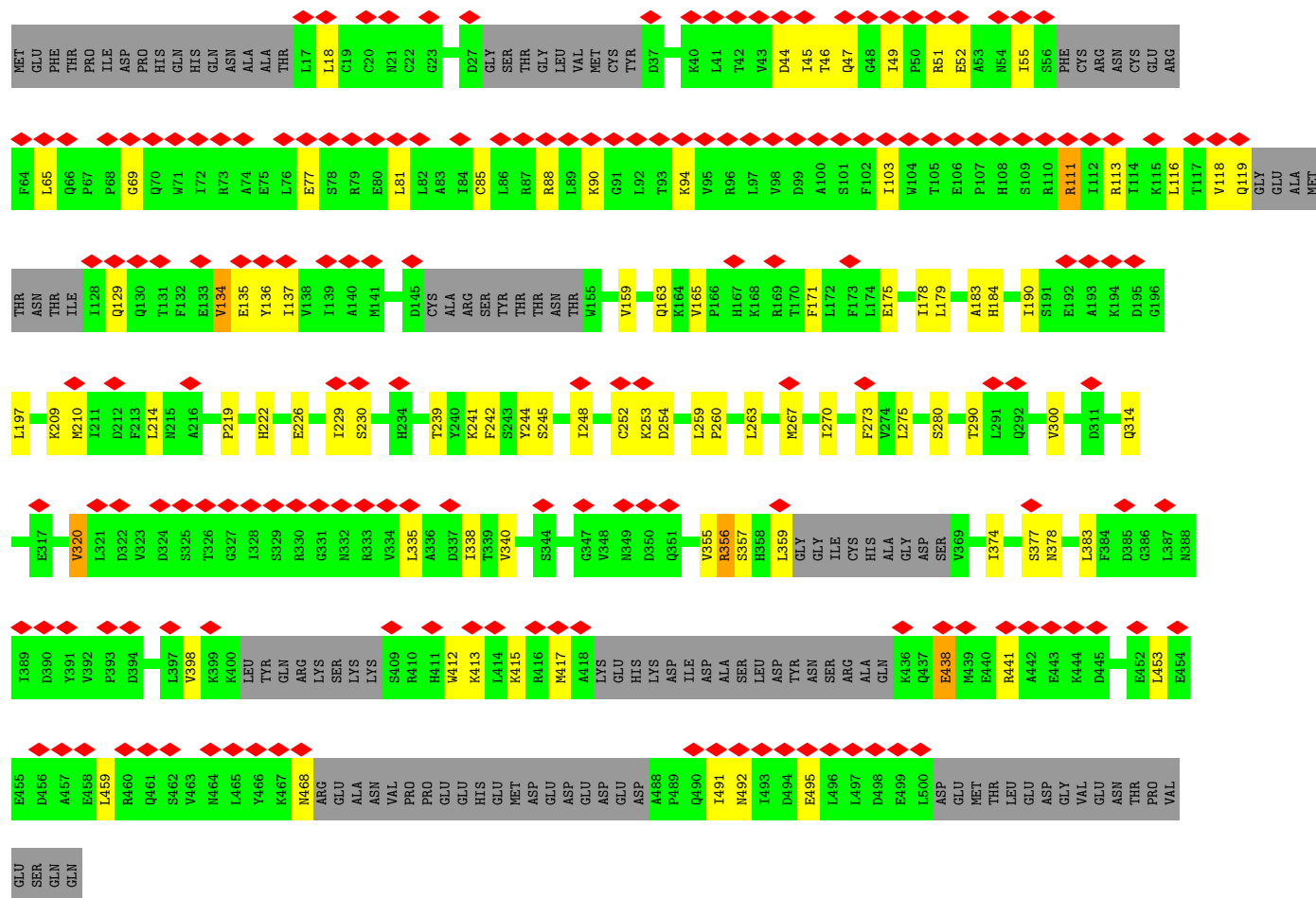
Chain X: 11% 69% 22% 8%



Chain W: 29% 38% 9% 24%



- Molecule 47: 60S ribosomal export protein NMD3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	99672	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 ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.750	Depositor
Minimum map value	-0.346	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	499.91998, 499.91998, 499.91998	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8332, 0.8332, 0.8332	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3HE

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	0.21	0/72400	0.38	2/112855 (0.0%)
2	B	0.18	0/2883	0.33	0/4491
3	C	0.20	0/3746	0.36	0/5832
4	z	0.25	0/472	0.58	0/626
5	LD	0.27	0/1908	0.65	2/2564 (0.1%)
6	LE	0.26	0/3152	0.56	0/4239
7	LF	0.24	0/2801	0.56	0/3792
8	LG	0.29	0/2347	0.71	1/3167 (0.0%)
9	LH	0.31	0/1265	0.74	0/1706
10	LI	0.26	0/1821	0.54	0/2451
11	LJ	0.26	0/1811	0.62	0/2445
12	LK	0.33	0/1514	0.74	0/2039
13	LL	0.26	0/1723	0.65	1/2312 (0.0%)
14	LM	0.30	0/1357	0.77	1/1818 (0.1%)
15	LN	0.28	0/1568	0.61	0/2106
16	LO	0.29	0/1068	0.63	0/1438
17	LP	0.25	0/1757	0.58	0/2354
18	LQ	0.28	0/1585	0.62	2/2128 (0.1%)
19	LR	0.27	0/1383	0.58	0/1858
20	LS	0.24	0/1465	0.52	0/1965
21	LT	0.24	0/1245	0.51	0/1661
22	LU	0.29	0/1473	0.63	0/1980
23	LV	0.27	0/1300	0.64	0/1743
24	LW	0.27	0/794	0.66	0/1076
25	LX	0.26	0/1018	0.62	0/1369
26	LY	0.26	0/525	0.57	0/696
27	LZ	0.27	0/974	0.61	0/1314
28	La	0.24	0/995	0.57	0/1329
29	Lb	0.28	0/1113	0.70	0/1490
30	Lc	0.25	0/1204	0.58	0/1612
31	Ld	0.28	0/473	0.71	1/629 (0.2%)
32	Le	0.33	0/745	0.80	0/1001

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Lf	0.27	0/870	0.59	0/1168
34	Lg	0.21	0/1033	0.50	0/1383
35	Lh	0.26	0/868	0.63	0/1168
36	Li	0.29	0/871	0.64	0/1164
37	Lj	0.29	0/978	0.68	0/1301
38	Lk	0.31	0/756	0.80	0/1005
39	Ll	0.25	0/660	0.63	0/875
40	Lm	0.28	0/610	0.68	0/815
41	Ln	0.29	0/443	0.66	0/588
42	Lo	0.24	0/407	0.62	0/540
43	Lq	0.29	0/813	0.69	1/1073 (0.1%)
44	Lr	0.26	0/701	0.62	0/934
45	X	0.37	0/1735	0.85	3/2360 (0.1%)
46	W	0.31	0/2460	0.78	1/3323 (0.0%)
47	V	0.32	0/3211	0.79	1/4344 (0.0%)
All	All	0.24	0/136301	0.50	16/200127 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	LE	0	4
8	LG	0	1
11	LJ	0	1
13	LL	0	5
15	LN	0	1
23	LV	0	2
25	LX	0	1
30	Lc	0	1
33	Lf	0	2
34	Lg	0	1
36	Li	0	1
43	Lq	0	1
45	X	0	2
46	W	0	3
47	V	0	1
All	All	0	27

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	X	93	LYS	CA-CB-CG	7.23	128.56	114.10
18	LQ	187	GLU	CA-CB-CG	6.40	126.89	114.10
45	X	85	ARG	CB-CG-CD	5.96	125.02	111.30
8	LG	263	GLU	CA-CB-CG	5.59	125.27	114.10
13	LL	117	GLY	N-CA-C	-5.45	100.28	113.18
1	A	2513	U	P-O3'-C3'	5.33	128.19	120.20
14	LM	131	MET	CB-CG-SD	5.31	128.63	112.70
31	Ld	47	LEU	CA-CB-CG	5.22	134.56	116.30
43	Lq	29	LYS	CB-CG-CD	5.17	123.20	111.30
5	LD	155	LYS	CA-CB-CG	5.17	124.43	114.10
5	LD	143	GLU	CB-CG-CD	5.15	121.36	112.60
45	X	95	GLN	CA-CB-CG	5.15	124.40	114.10
46	W	312	GLN	CA-CB-CG	5.11	124.32	114.10
1	A	1307	G	P-O3'-C3'	5.09	127.84	120.20
18	LQ	187	GLU	CB-CG-CD	5.07	121.23	112.60
47	V	438	GLU	CA-CB-CG	5.02	124.14	114.10

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	LE	332	ARG	Sidechain
6	LE	348	ARG	Sidechain
6	LE	369	ARG	Sidechain
6	LE	62	ARG	Sidechain
8	LG	54	ARG	Sidechain
11	LJ	249	ARG	Sidechain
13	LL	116	ARG	Sidechain
13	LL	153	ARG	Sidechain
13	LL	178	ARG	Sidechain
13	LL	211	ARG	Sidechain
13	LL	24	ARG	Sidechain
15	LN	188	ARG	Sidechain
23	LV	102	ARG	Sidechain
23	LV	108	ARG	Sidechain
25	LX	70	ARG	Sidechain
30	Lc	42	ARG	Sidechain
33	Lf	50	ARG	Sidechain
33	Lf	79	ARG	Sidechain
34	Lg	125	ARG	Sidechain
36	Li	88	ARG	Sidechain
43	Lq	80	ARG	Sidechain
47	V	356	ARG	Sidechain

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Mol	Chain	Res	Type	Group
46	W	138	ARG	Sidechain
46	W	164	ARG	Sidechain
46	W	208	ARG	Sidechain
45	X	61	ARG	Sidechain
45	X	68	ARG	Sidechain

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	64684	0	32516	330	0
2	B	2579	0	1304	15	0
3	C	3353	0	1695	10	0
4	z	469	0	492	9	0
5	LD	1874	0	1943	33	0
6	LE	3081	0	3165	36	0
7	LF	2749	0	2863	24	0
8	LG	2298	0	2251	23	0
9	LH	1243	0	1327	11	0
10	LI	1784	0	1862	14	0
11	LJ	1780	0	1865	13	0
12	LK	1493	0	1566	31	0
13	LL	1686	0	1725	20	0
14	LM	1336	0	1370	27	0
15	LN	1543	0	1608	20	0
16	LO	1053	0	1149	10	0
17	LP	1720	0	1779	21	0
18	LQ	1555	0	1659	12	0
19	LR	1361	0	1398	17	0
20	LS	1441	0	1543	15	0
21	LT	1228	0	1314	5	0
22	LU	1437	0	1475	18	0
23	LV	1276	0	1323	15	0
24	LW	778	0	791	7	0
25	LX	1003	0	1048	15	0
26	LY	513	0	540	6	0
27	LZ	959	0	1023	10	0
28	La	984	0	1075	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	Lb	1087	0	1150	15	0
30	Lc	1173	0	1215	18	0
31	Ld	462	0	491	2	0
32	Le	737	0	792	14	0
33	Lf	856	0	904	6	0
34	Lg	1012	0	1079	8	0
35	Lh	850	0	880	8	0
36	Li	861	0	922	3	0
37	Lj	969	0	1078	15	0
38	Lk	750	0	829	14	0
39	Ll	645	0	647	3	0
40	Lm	604	0	671	5	0
41	Ln	436	0	475	8	0
42	Lo	401	0	437	6	0
43	Lq	801	0	874	14	0
44	Lr	694	0	738	6	0
45	X	1713	0	1699	46	0
46	W	2417	0	2469	36	0
47	V	3159	0	3153	52	0
48	A	20	0	23	0	0
All	All	126907	0	94195	946	0

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

All (946) 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)
1:A:3348:G:H1	1:A:3357:U:H3	1.09	0.92
1:A:2193:U:H5'	1:A:2194:G:H5'	1.64	0.80
46:W:139:ARG:HH22	46:W:196:GLU:HB2	1.48	0.77
25:LX:132:ASN:HD21	45:X:192:PHE:HZ	1.31	0.74
5:LD:104:LEU:HD12	5:LD:158:ILE:HD11	1.70	0.74
14:LM:37:LEU:HD13	14:LM:69:VAL:HG12	1.69	0.73
47:V:55:ILE:HD11	47:V:136:TYR:HD1	1.53	0.72
12:LK:92:TYR:HB3	12:LK:99:ILE:HD11	1.70	0.71
1:A:3243:A:H4'	6:LE:95:THR:HG22	1.71	0.71
12:LK:9:GLN:HB3	12:LK:52:LEU:HD21	1.72	0.71
5:LD:135:ILE:HG23	5:LD:149:ARG:HB3	1.73	0.70
1:A:1949:G:H1	1:A:2097:U:H3	1.39	0.70
1:A:3165:A:H61	1:A:3285:C:H42	1.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:X:85:ARG:HA	45:X:85:ARG:HH11	1.55	0.70
47:V:438:GLU:HB2	47:V:441:ARG:HH21	1.58	0.69
47:V:119:GLN:HG2	47:V:129:GLN:HG2	1.75	0.69
1:A:2514:U:H5'	11:LJ:68:ARG:HG3	1.75	0.68
22:LU:82:ASP:HB2	22:LU:120:SER:HB2	1.76	0.68
45:X:148:VAL:O	45:X:152:CYS:CB	2.42	0.68
45:X:22:THR:HG23	45:X:67:ARG:HG2	1.75	0.68
41:Ln:21:ARG:HH21	41:Ln:24:PRO:HB3	1.58	0.68
47:V:229:ILE:HD11	47:V:241:LYS:HB2	1.75	0.67
1:A:2270:A:H2'	1:A:2271:A:C8	2.29	0.67
12:LK:4:ILE:H	22:LU:142:GLN:HE22	1.40	0.67
1:A:2421:U:H4'	43:Lq:53:GLN:HB2	1.75	0.66
6:LE:82:PRO:HG3	6:LE:319:ASN:HD22	1.60	0.66
28:La:55:GLU:HG3	28:La:108:LYS:HB3	1.77	0.66
7:LF:170:LYS:HG3	7:LF:175:HIS:HB2	1.78	0.65
8:LG:211:LEU:HB3	8:LG:219:PHE:HB2	1.78	0.65
45:X:142:ILE:HG22	45:X:148:VAL:HG12	1.79	0.65
40:Lm:42:LYS:HG2	40:Lm:55:VAL:HG22	1.78	0.65
6:LE:229:VAL:HG11	6:LE:249:VAL:HG23	1.78	0.64
15:LN:48:PRO:HA	15:LN:137:GLN:HB2	1.79	0.64
22:LU:77:VAL:HG12	22:LU:126:VAL:HG22	1.80	0.63
12:LK:1:MET:HG3	22:LU:139:TYR:HB3	1.80	0.63
29:Lb:54:THR:HG22	29:Lb:56:LYS:H	1.63	0.63
45:X:148:VAL:O	45:X:152:CYS:HB2	1.98	0.63
3:C:135:G:H5''	27:LZ:49:LYS:HD2	1.81	0.63
1:A:3160:U:H3	1:A:3290:G:H1	1.45	0.63
7:LF:233:LEU:HD13	7:LF:238:LEU:HD11	1.81	0.63
1:A:655:C:H2'	1:A:656:A:H8	1.64	0.63
47:V:111:ARG:HH12	47:V:137:ILE:HG12	1.63	0.63
47:V:190:ILE:HD13	47:V:417:MET:HE3	1.81	0.62
29:Lb:81:LEU:HD22	36:Li:90:ILE:HD13	1.82	0.62
1:A:3358:U:H2'	1:A:3359:A:H8	1.64	0.62
25:LX:54:LEU:HD11	25:LX:119:GLY:HA3	1.81	0.62
1:A:2424:A:H61	5:LD:230:VAL:HG11	1.65	0.61
1:A:2418:G:H22	47:V:300:VAL:HA	1.66	0.61
11:LJ:82:LEU:HD21	11:LJ:178:ALA:HB1	1.81	0.61
27:LZ:110:VAL:HG22	27:LZ:124:VAL:HG13	1.82	0.61
46:W:160:LEU:HB3	46:W:164:ARG:HH12	1.64	0.61
29:Lb:15:ARG:HD2	29:Lb:79:HIS:HD2	1.65	0.60
46:W:461:LEU:HD13	46:W:480:GLU:HB3	1.82	0.60
17:LP:110:ALA:HB1	17:LP:113:LEU:HD23	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:LM:40:LEU:HD12	14:LM:114:ILE:HD11	1.82	0.60
43:Lq:90:HIS:HB2	47:V:314:GLN:HE22	1.65	0.60
14:LM:110:ILE:HA	14:LM:114:ILE:HB	1.83	0.60
18:LQ:10:ASP:HB2	18:LQ:117:ARG:HB3	1.82	0.60
47:V:49:ILE:HG22	47:V:51:ARG:H	1.66	0.60
15:LN:123:ILE:HG22	37:Lj:118:ILE:HG22	1.82	0.60
24:LW:15:PHE:HB2	24:LW:65:VAL:HG13	1.83	0.60
25:LX:39:VAL:HG23	25:LX:58:VAL:HG12	1.83	0.60
28:La:45:ILE:HD13	28:La:119:ILE:HG23	1.83	0.60
45:X:142:ILE:HD11	45:X:162:HIS:H	1.67	0.59
6:LE:92:TYR:HB2	6:LE:157:VAL:HG13	1.84	0.59
45:X:4:ARG:HG3	45:X:208:LEU:HA	1.85	0.59
30:Lc:130:VAL:HG11	30:Lc:145:VAL:HG11	1.84	0.59
1:A:585:A:H4'	35:Lh:72:THR:HG22	1.84	0.59
14:LM:60:ARG:HB3	14:LM:63:GLU:HB2	1.83	0.59
19:LR:13:LYS:HB3	19:LR:152:GLU:HG3	1.83	0.59
21:LT:105:LEU:HD13	21:LT:135:LYS:HE3	1.83	0.59
1:A:2357:A:H2'	1:A:2358:A:H8	1.67	0.59
45:X:72:VAL:HB	45:X:76:THR:HG21	1.85	0.59
1:A:68:C:H41	1:A:315:C:H5'	1.68	0.59
29:Lb:70:PRO:HG3	29:Lb:115:LYS:HB2	1.85	0.59
6:LE:152:LYS:HG2	6:LE:192:VAL:HG21	1.84	0.58
12:LK:41:ILE:HG22	12:LK:43:VAL:HG13	1.86	0.58
29:Lb:3:LYS:HB2	29:Lb:6:LYS:HZ1	1.69	0.58
40:Lm:66:ILE:HA	40:Lm:69:LEU:HD12	1.84	0.58
47:V:263:LEU:HG	47:V:267:MET:HE2	1.86	0.58
7:LF:35:VAL:HG21	7:LF:244:LEU:HD21	1.84	0.58
13:LL:42:THR:HG22	13:LL:44:ASP:H	1.67	0.58
47:V:178:ILE:HG23	47:V:183:ALA:HB3	1.85	0.58
1:A:44:U:H1'	43:Lq:54:THR:HG23	1.86	0.58
11:LJ:186:LEU:HB3	11:LJ:195:SER:HB3	1.84	0.58
29:Lb:90:GLU:HA	29:Lb:93:LYS:HE3	1.85	0.58
45:X:170:GLN:HE22	45:X:183:ALA:HB2	1.67	0.58
1:A:2656:A:H4'	43:Lq:98:LYS:HE2	1.86	0.58
1:A:1661:G:H2'	1:A:1662:G:C8	2.39	0.57
13:LL:86:HIS:HB3	13:LL:139:ARG:HG2	1.86	0.57
37:Lj:4:VAL:HG22	37:Lj:50:SER:HB2	1.86	0.57
4:z:416:GLU:O	4:z:420:VAL:HB	2.04	0.57
12:LK:147:SER:HB2	12:LK:187:ILE:HD11	1.87	0.57
1:A:1639:C:H5'	36:Li:52:GLN:HG2	1.85	0.57
28:La:48:LEU:HD13	28:La:115:ARG:HH21	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:LR:124:LYS:HB2	19:LR:140:GLU:HB3	1.87	0.57
44:Lr:30:GLU:HA	44:Lr:33:GLN:HG2	1.87	0.57
17:LP:37:HIS:CD2	17:LP:63:ARG:HB3	2.40	0.56
1:A:1168:U:H2'	1:A:1169:A:H8	1.70	0.56
6:LE:43:LEU:HD22	6:LE:181:ILE:HD11	1.87	0.56
32:Le:30:THR:HG21	32:Le:89:VAL:HG23	1.87	0.56
8:LG:287:ALA:HA	8:LG:290:ILE:HD12	1.87	0.56
47:V:492:ASN:HB2	47:V:495:GLU:HG3	1.87	0.56
7:LF:136:LEU:HD21	7:LF:143:GLU:HG3	1.87	0.56
19:LR:114:VAL:HG12	19:LR:150:VAL:HG12	1.87	0.56
45:X:104:LEU:HA	45:X:107:VAL:HG22	1.87	0.56
1:A:597:G:H2'	1:A:598:A:H8	1.70	0.56
43:Lq:47:GLN:HE22	43:Lq:53:GLN:HE22	1.53	0.56
6:LE:278:ILE:HG13	6:LE:279:ASN:HD22	1.71	0.56
1:A:2364:G:H22	1:A:2396:G:H1'	1.71	0.55
1:A:500:C:H4'	9:LH:80:ASN:HD21	1.71	0.55
8:LG:132:THR:HG21	8:LG:170:GLY:HA2	1.88	0.55
1:A:700:C:H2'	1:A:701:G:H8	1.71	0.55
1:A:2597:U:H2'	1:A:2598:G:H8	1.72	0.55
13:LL:36:LEU:HD21	13:LL:69:ARG:HD2	1.89	0.55
13:LL:54:SER:HB2	13:LL:135:ILE:HD11	1.89	0.55
1:A:2344:U:H2'	1:A:2345:A:H8	1.72	0.55
12:LK:41:ILE:HG21	12:LK:71:VAL:HG21	1.87	0.55
1:A:571:U:H2'	1:A:572:A:H8	1.71	0.55
29:Lb:15:ARG:HD2	29:Lb:79:HIS:CD2	2.41	0.55
15:LN:47:ALA:HB1	15:LN:48:PRO:HD2	1.88	0.55
24:LW:81:LYS:HD2	24:LW:90:ARG:HH11	1.71	0.55
37:Lj:104:GLN:O	37:Lj:108:GLN:HG3	2.07	0.55
8:LG:30:TYR:HA	8:LG:33:ARG:HB2	1.88	0.55
1:A:1786:G:H2'	1:A:1787:A:C8	2.42	0.55
1:A:2351:U:H2'	1:A:2352:A:H8	1.72	0.55
5:LD:136:ILE:HD13	5:LD:148:VAL:HG12	1.89	0.55
23:LV:14:MET:HE2	23:LV:58:GLN:HB3	1.88	0.55
1:A:2413:A:H2'	1:A:2414:G:H8	1.72	0.55
1:A:2768:U:H2'	1:A:2769:A:H8	1.72	0.54
7:LF:11:LEU:HD21	7:LF:156:LEU:HB2	1.89	0.54
12:LK:115:ARG:HG2	12:LK:123:ILE:HG23	1.89	0.54
47:V:230:SER:OG	47:V:239:THR:HG22	2.07	0.54
25:LX:128:ARG:NH2	45:X:192:PHE:CE2	2.76	0.54
45:X:148:VAL:O	45:X:152:CYS:HB3	2.06	0.54
46:W:135:ILE:HG22	46:W:162:TRP:HD1	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:LF:362:ASP:HA	22:LU:28:ARG:HH11	1.73	0.54
14:LM:76:ALA:HA	14:LM:79:ILE:HD12	1.89	0.54
45:X:126:GLU:HA	45:X:137:VAL:HG21	1.88	0.54
45:X:85:ARG:HA	45:X:85:ARG:NH1	2.23	0.54
1:A:1576:G:H2'	1:A:1577:G:C8	2.42	0.54
9:LH:43:LEU:HD11	9:LH:85:ILE:HD11	1.90	0.54
1:A:1497:C:H2'	1:A:1498:A:H8	1.73	0.54
14:LM:13:LYS:HD3	14:LM:134:PRO:HG3	1.89	0.54
17:LP:64:VAL:HG11	17:LP:102:ALA:HB1	1.88	0.54
46:W:177:LEU:HD22	46:W:399:ASN:HA	1.89	0.54
47:V:453:LEU:HD12	47:V:459:LEU:HB3	1.90	0.54
1:A:2225:U:H4'	43:Lq:36:PHE:HZ	1.72	0.54
18:LQ:61:ALA:HA	18:LQ:70:PRO:HD2	1.90	0.54
1:A:3255:U:H2'	1:A:3256:G:H8	1.73	0.54
12:LK:20:ILE:HG12	12:LK:25:VAL:HG22	1.90	0.54
1:A:728:G:H5''	20:LS:43:PRO:HB2	1.90	0.53
1:A:3358:U:H2'	1:A:3359:A:C8	2.41	0.53
12:LK:27:VAL:HG12	12:LK:82:VAL:HG21	1.90	0.53
27:LZ:107:VAL:HA	27:LZ:126:LEU:HA	1.91	0.53
1:A:1805:C:H2'	1:A:1806:A:H8	1.73	0.53
10:LI:121:LYS:HB2	23:LV:133:ALA:HB3	1.89	0.53
17:LP:187:ARG:HG2	17:LP:187:ARG:HH11	1.73	0.53
29:Lb:50:PRO:HD3	29:Lb:68:ILE:HG22	1.91	0.53
1:A:2262:A:H5'	1:A:2262:A:H8	1.73	0.53
12:LK:114:VAL:HB	12:LK:124:ARG:HG3	1.90	0.53
37:Lj:28:LEU:HD13	37:Lj:32:LYS:HE2	1.90	0.53
2:B:7:G:H5''	8:LG:22:ARG:HD3	1.90	0.53
14:LM:109:HIS:HD2	14:LM:123:PHE:H	1.57	0.53
17:LP:39:ALA:HB3	17:LP:61:ILE:HG13	1.90	0.53
32:Le:49:PRO:HG2	32:Le:52:ARG:HB3	1.89	0.53
1:A:1576:G:H2'	1:A:1577:G:H8	1.72	0.53
1:A:2561:A:C2	11:LJ:32:LYS:HG3	2.44	0.53
1:A:3015:G:H2'	1:A:3016:A:H8	1.74	0.53
5:LD:101:VAL:HG22	5:LD:165:VAL:HG22	1.90	0.53
15:LN:9:ILE:HD11	30:Lc:45:MET:HE1	1.90	0.53
15:LN:166:ALA:HB1	30:Lc:147:LEU:HD21	1.91	0.53
1:A:3233:C:H2'	1:A:3234:A:C8	2.44	0.53
14:LM:29:ARG:HB3	14:LM:123:PHE:HZ	1.73	0.53
33:Lf:36:ILE:HD12	33:Lf:59:ILE:HD11	1.90	0.53
1:A:1119:C:H2'	1:A:1120:A:H8	1.74	0.53
25:LX:45:ARG:HD3	25:LX:46:LEU:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:83:C:H1'	3:C:85:G:H21	1.75	0.52
7:LF:142:VAL:HA	7:LF:145:ILE:HD13	1.90	0.52
1:A:2697:A:H2'	1:A:2698:G:C8	2.44	0.52
45:X:162:HIS:CD2	45:X:191:SER:HB3	2.44	0.52
4:z:381:ALA:O	4:z:385:MET:HG3	2.10	0.52
12:LK:162:GLN:HE21	12:LK:180:TYR:HA	1.75	0.52
27:LZ:117:ASN:HB2	41:Ln:18:LYS:HE3	1.91	0.52
47:V:94:LYS:HD3	47:V:118:VAL:HG12	1.92	0.52
1:A:1411:C:H2'	1:A:1412:G:H8	1.74	0.52
4:z:421:ASN:HD21	19:LR:136:ILE:H	1.56	0.52
29:Lb:23:VAL:HG12	29:Lb:45:GLY:HA3	1.91	0.52
1:A:594:U:H3	7:LF:304:GLN:HE22	1.58	0.52
18:LQ:75:ALA:HB3	18:LQ:78:ARG:HG2	1.91	0.52
1:A:105:C:H2'	1:A:106:A:H8	1.73	0.52
1:A:155:G:H21	38:Lk:26:ILE:HD11	1.75	0.52
1:A:821:U:H2'	1:A:822:G:H8	1.74	0.52
1:A:1097:G:H5'	23:LV:129:LYS:HE2	1.92	0.52
1:A:3023:U:H2'	1:A:3024:A:H8	1.75	0.52
41:Ln:24:PRO:HG2	41:Ln:27:ILE:HD12	1.91	0.52
5:LD:112:ILE:HG13	44:Lr:79:VAL:HG22	1.91	0.52
12:LK:167:VAL:HB	12:LK:172:ILE:HG22	1.92	0.52
29:Lb:25:ILE:HG22	29:Lb:43:VAL:HG12	1.90	0.52
1:A:3016:A:H2'	1:A:3017:A:H8	1.75	0.51
14:LM:109:HIS:CD2	14:LM:123:PHE:H	2.28	0.51
45:X:71:LEU:HD21	45:X:132:VAL:HG11	1.91	0.51
3:C:8:C:H2'	3:C:9:A:H8	1.75	0.51
25:LX:59:MET:HE1	25:LX:75:PRO:HG3	1.92	0.51
35:Lh:39:GLN:H	35:Lh:39:GLN:NE2	2.08	0.51
46:W:151:LEU:O	46:W:155:GLU:HG2	2.09	0.51
6:LE:60:LEU:HD13	6:LE:62:ARG:H	1.74	0.51
1:A:655:C:H2'	1:A:656:A:C8	2.44	0.51
1:A:2960:C:H2'	1:A:2961:G:C8	2.45	0.51
22:LU:80:ARG:HG2	22:LU:124:LEU:HD11	1.92	0.51
46:W:181:PHE:HB3	46:W:394:PRO:HD3	1.92	0.51
1:A:50:U:H2'	1:A:51:A:H8	1.76	0.51
1:A:664:U:H2'	1:A:665:A:C8	2.46	0.51
1:A:1497:C:H2'	1:A:1498:A:C8	2.46	0.51
13:LL:190:VAL:O	13:LL:191:LYS:HD2	2.10	0.51
5:LD:117:GLU:HB2	5:LD:162:ALA:HB1	1.92	0.51
33:Lf:55:LEU:HB2	33:Lf:95:PRO:HD3	1.92	0.51
41:Ln:26:TRP:HA	41:Ln:29:LEU:HD23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:Ln:27:ILE:HA	41:Ln:30:ARG:HD3	1.92	0.51
46:W:200:LEU:HB3	46:W:339:ILE:HG22	1.92	0.51
2:B:29:C:H2'	2:B:51:A:H61	1.75	0.51
5:LD:47:GLN:HE21	5:LD:49:VAL:HG11	1.75	0.51
46:W:202:VAL:HA	46:W:232:LEU:O	2.11	0.51
1:A:1203:A:H2'	1:A:1204:A:C8	2.46	0.51
28:La:115:ARG:O	28:La:119:ILE:HG13	2.10	0.51
28:La:119:ILE:HG22	28:La:124:GLY:HA3	1.91	0.51
7:LF:350:LYS:HG3	7:LF:351:PRO:HD2	1.91	0.51
31:Ld:32:LEU:HD22	31:Ld:35:VAL:HG21	1.92	0.51
45:X:32:GLU:HA	45:X:35:TYR:HD2	1.76	0.51
1:A:370:U:H4'	1:A:404:G:H5'	1.93	0.51
11:LJ:249:ARG:HG2	11:LJ:249:ARG:HH11	1.75	0.51
23:LV:100:LYS:HD2	23:LV:103:GLN:HG3	1.93	0.51
33:Lf:20:LEU:HD13	33:Lf:28:ARG:HG3	1.92	0.51
38:Lk:79:SER:HB3	38:Lk:82:ARG:HG3	1.91	0.51
1:A:1799:A:H2'	1:A:1800:A:H8	1.76	0.50
2:B:56:A:H4'	14:LM:152:HIS:HB2	1.93	0.50
25:LX:131:SER:HB2	45:X:192:PHE:CE1	2.46	0.50
32:Le:16:LEU:HD21	32:Le:97:ASP:HB2	1.92	0.50
45:X:58:ILE:O	45:X:62:MET:HG2	2.11	0.50
1:A:3119:U:H4'	42:Lo:104:PRO:HG2	1.93	0.50
2:B:121:U:C2	8:LG:268:GLU:HG3	2.47	0.50
7:LF:188:ARG:HD2	7:LF:192:GLY:HA3	1.94	0.50
12:LK:57:VAL:HG13	12:LK:68:LEU:HD23	1.92	0.50
34:Lg:89:THR:HG22	34:Lg:117:ILE:HG13	1.93	0.50
1:A:2254:U:H3'	1:A:2259:A:H61	1.76	0.50
1:A:2433:U:H1'	17:LP:125:SER:HB3	1.94	0.50
12:LK:89:LYS:HG2	12:LK:145:VAL:HG22	1.93	0.50
12:LK:92:TYR:HD1	12:LK:179:ILE:HG23	1.75	0.50
47:V:275:LEU:HD11	47:V:398:VAL:HG12	1.93	0.50
4:z:380:ALA:O	4:z:384:ARG:HG3	2.11	0.50
10:LI:224:ILE:HD11	22:LU:35:VAL:HG12	1.94	0.50
1:A:307:A:H2'	1:A:308:A:C8	2.47	0.50
1:A:1717:U:H2'	1:A:1718:G:C8	2.46	0.50
1:A:3255:U:H2'	1:A:3256:G:C8	2.46	0.50
7:LF:8:VAL:HA	7:LF:151:VAL:HG13	1.92	0.50
4:z:397:GLY:O	4:z:401:MET:HG2	2.12	0.50
38:Lk:43:LEU:O	38:Lk:47:ILE:HG13	2.12	0.50
14:LM:29:ARG:HG2	14:LM:32:ARG:HH21	1.77	0.50
46:W:137:PRO:HB2	46:W:192:TRP:HZ2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2253:G:H1	1:A:2263:C:H5	1.59	0.50
9:LH:132:THR:HA	9:LH:135:VAL:HG12	1.92	0.50
20:LS:178:ARG:HG2	30:Lc:51:GLY:HA3	1.94	0.50
7:LF:8:VAL:HG13	7:LF:16:THR:HG23	1.94	0.49
13:LL:48:LEU:HD21	13:LL:145:LYS:HD3	1.94	0.49
25:LX:108:GLU:HA	25:LX:128:ARG:HG3	1.93	0.49
45:X:63:THR:HG22	45:X:72:VAL:HA	1.93	0.49
46:W:377:ILE:HD12	46:W:385:LEU:HB2	1.93	0.49
45:X:97:VAL:HG23	45:X:128:LEU:HD13	1.94	0.49
1:A:289:A:H2'	1:A:290:G:H8	1.78	0.49
45:X:186:VAL:HG21	45:X:197:MET:HG2	1.93	0.49
1:A:1799:A:H2'	1:A:1800:A:C8	2.47	0.49
1:A:3333:G:H22	1:A:3369:G:H1'	1.78	0.49
12:LK:77:ASN:HB3	12:LK:151:VAL:HG21	1.94	0.49
45:X:84:LEU:O	45:X:88:LEU:HB2	2.13	0.49
1:A:786:A:H4'	1:A:787:G:H5'	1.94	0.49
1:A:1336:U:H2'	1:A:1337:A:H8	1.78	0.49
32:Le:51:LEU:HD11	36:Li:90:ILE:HG22	1.94	0.49
37:Lj:78:LYS:HA	37:Lj:81:ARG:HD3	1.94	0.49
42:Lo:99:CYS:HB3	42:Lo:115:CYS:HB3	1.94	0.49
1:A:567:G:H2'	1:A:568:G:C8	2.48	0.49
1:A:753:C:H2'	1:A:754:G:H8	1.77	0.49
10:LI:80:GLN:HB2	23:LV:135:PRO:HB2	1.93	0.49
17:LP:109:ARG:HG2	17:LP:109:ARG:HH11	1.77	0.49
1:A:903:U:H2'	1:A:904:A:H8	1.78	0.49
1:A:2949:U:H4'	6:LE:241:LYS:HD3	1.93	0.49
8:LG:243:ALA:O	8:LG:247:ILE:HG13	2.12	0.49
14:LM:31:THR:HG22	14:LM:35:LYS:HE3	1.95	0.49
46:W:185:ILE:HG12	46:W:189:LYS:NZ	2.28	0.49
1:A:2812:C:H2'	1:A:2813:A:C8	2.48	0.49
1:A:3006:A:H62	1:A:3140:G:H21	1.61	0.49
1:A:3121:U:H1'	1:A:3122:A:H5''	1.95	0.49
15:LN:64:LYS:HE3	15:LN:65:TYR:CZ	2.48	0.49
16:LO:15:VAL:HG23	16:LO:35:ILE:HD13	1.93	0.49
23:LV:89:LEU:HD13	23:LV:91:LEU:HD11	1.94	0.49
29:Lb:101:PHE:HA	29:Lb:107:ARG:HE	1.78	0.49
7:LF:281:ILE:HG13	20:LS:125:ASP:OD1	2.13	0.49
14:LM:166:LYS:HG2	14:LM:167:TYR:CD1	2.48	0.49
32:Le:31:VAL:O	32:Le:35:ARG:HB2	2.13	0.49
45:X:93:LYS:NZ	45:X:95:GLN:HB2	2.28	0.49
13:LL:91:VAL:HG12	13:LL:133:GLN:HE21	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:LQ:27:LEU:HD11	18:LQ:102:LEU:HB2	1.94	0.48
25:LX:131:SER:HB2	45:X:192:PHE:HE1	1.75	0.48
47:V:273:PHE:HE2	47:V:374:ILE:HD13	1.78	0.48
1:A:312:C:H2'	1:A:313:A:H8	1.77	0.48
1:A:3322:A:H2'	1:A:3323:A:C8	2.48	0.48
5:LD:2:GLY:HA2	5:LD:207:VAL:HG23	1.94	0.48
15:LN:37:ASN:O	15:LN:41:THR:HG23	2.14	0.48
1:A:411:U:H2'	1:A:412:G:H8	1.78	0.48
1:A:2263:C:H2'	1:A:2264:U:C6	2.48	0.48
5:LD:92:LYS:HG2	5:LD:93:LYS:HD2	1.95	0.48
46:W:183:ARG:HD3	47:V:77:GLU:HG2	1.94	0.48
10:LI:176:TYR:CZ	10:LI:197:GLN:HG2	2.48	0.48
24:LW:38:ILE:HD12	24:LW:38:ILE:H	1.78	0.48
47:V:90:LYS:HZ2	47:V:94:LYS:HB3	1.78	0.48
1:A:68:C:N4	1:A:315:C:H5'	2.28	0.48
12:LK:174:LYS:HD3	42:Lo:127:LEU:HD21	1.95	0.48
14:LM:74:PRO:HA	14:LM:77:GLU:HG3	1.94	0.48
15:LN:36:ARG:HG2	15:LN:39:ARG:HH21	1.79	0.48
29:Lb:60:LYS:H	29:Lb:60:LYS:HD2	1.78	0.48
1:A:3034:C:C2	12:LK:120:ASP:HB3	2.49	0.48
1:A:528:U:H2'	1:A:529:A:C8	2.49	0.48
1:A:1084:A:H2'	1:A:1085:A:C8	2.49	0.48
1:A:3357:U:H2'	1:A:3358:U:C6	2.49	0.48
1:A:3016:A:H2'	1:A:3017:A:C8	2.49	0.48
1:A:3348:G:O6	1:A:3357:U:O4	2.32	0.48
39:Ll:24:ARG:HE	39:Ll:24:ARG:HB3	1.50	0.48
46:W:427:ARG:HG3	46:W:427:ARG:HH11	1.79	0.48
1:A:3313:U:H4'	6:LE:173:GLN:HG3	1.96	0.48
3:C:8:C:H2'	3:C:9:A:C8	2.49	0.48
1:A:1553:U:H4'	1:A:1554:U:H5'	1.95	0.48
3:C:21:C:H5''	7:LF:194:TYR:HE1	1.78	0.48
7:LF:208:VAL:HG22	7:LF:228:ALA:HB3	1.96	0.48
20:LS:70:ALA:HB1	20:LS:138:LEU:HD21	1.96	0.48
1:A:2160:G:H2'	1:A:2161:G:H8	1.78	0.47
1:A:2228:A:H2'	1:A:2229:A:C8	2.49	0.47
7:LF:60:THR:HG21	7:LF:84:ARG:HH21	1.77	0.47
18:LQ:62:THR:HG23	18:LQ:69:GLY:HA2	1.94	0.47
19:LR:124:LYS:HA	19:LR:143:PRO:HD3	1.95	0.47
25:LX:84:SER:HA	25:LX:94:TYR:HB3	1.96	0.47
47:V:163:GLN:HB2	47:V:248:ILE:HB	1.94	0.47
45:X:192:PHE:HB3	45:X:195:ALA:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2571:U:H1'	1:A:2572:C:H2'	1.95	0.47
1:A:2960:C:H2'	1:A:2961:G:H8	1.80	0.47
7:LF:286:VAL:HG11	20:LS:31:LYS:HD2	1.96	0.47
23:LV:39:ILE:HD13	23:LV:63:VAL:HG22	1.96	0.47
37:Lj:101:THR:HG22	37:Lj:104:GLN:HG2	1.97	0.47
46:W:341:LEU:HD11	46:W:385:LEU:HD12	1.94	0.47
1:A:1777:U:H2'	1:A:1778:G:C8	2.48	0.47
1:A:2357:A:H2'	1:A:2358:A:C8	2.48	0.47
1:A:2953:U:H2'	1:A:2954:U:H2'	1.97	0.47
8:LG:270:LYS:HG2	8:LG:273:ARG:HE	1.79	0.47
12:LK:162:GLN:NE2	12:LK:180:TYR:HA	2.29	0.47
15:LN:63:VAL:HA	15:LN:66:ASN:HB2	1.95	0.47
27:LZ:62:VAL:HG23	27:LZ:63:ILE:HG13	1.95	0.47
37:Lj:21:LEU:HB2	37:Lj:54:VAL:HG11	1.96	0.47
1:A:1666:G:H2'	1:A:1667:A:H8	1.78	0.47
1:A:2186:U:H5	5:LD:200:ARG:HD3	1.79	0.47
1:A:3107:U:H2'	1:A:3108:G:C8	2.50	0.47
12:LK:101:VAL:HA	12:LK:113:GLU:O	2.15	0.47
47:V:259:LEU:HD13	47:V:267:MET:HE3	1.95	0.47
12:LK:112:ILE:HD11	12:LK:134:ILE:HG13	1.96	0.47
1:A:54:C:H2'	1:A:55:G:H8	1.79	0.47
1:A:298:U:H5'	38:Lk:32:ALA:HA	1.97	0.47
1:A:1798:A:H2'	1:A:1799:A:C8	2.50	0.47
1:A:2376:G:H2'	1:A:2377:G:C8	2.50	0.47
1:A:2676:A:H5'	1:A:2677:G:C8	2.50	0.47
1:A:2812:C:H2'	1:A:2813:A:H8	1.80	0.47
8:LG:25:GLU:HG3	8:LG:27:LYS:HG3	1.97	0.47
8:LG:122:VAL:HG22	8:LG:124:GLU:O	2.15	0.47
8:LG:146:LEU:HD22	8:LG:163:LEU:HD22	1.95	0.47
14:LM:29:ARG:HG2	14:LM:32:ARG:NH2	2.30	0.47
19:LR:46:LYS:O	19:LR:50:GLN:HG3	2.15	0.47
27:LZ:115:ARG:HD2	27:LZ:121:LYS:HD2	1.96	0.47
28:La:39:LEU:HG	28:La:43:TYR:HE2	1.80	0.47
43:Lq:47:GLN:HE22	43:Lq:53:GLN:NE2	2.13	0.47
46:W:137:PRO:HB2	46:W:192:TRP:CZ2	2.50	0.47
46:W:247:ILE:O	46:W:251:LYS:HG2	2.14	0.47
47:V:335:LEU:HB3	47:V:356:ARG:HH22	1.80	0.47
1:A:1564:U:H3'	1:A:1565:G:C8	2.49	0.47
6:LE:214:MET:HE2	6:LE:350:ALA:HA	1.97	0.47
13:LL:140:THR:HG21	13:LL:148:VAL:HG21	1.97	0.47
17:LP:181:ASN:HA	17:LP:184:LYS:HE3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:LZ:135:ILE:O	27:LZ:139:ILE:HG12	2.15	0.47
14:LM:49:LYS:HG3	14:LM:64:LYS:HG3	1.96	0.47
47:V:222:HIS:HA	47:V:245:SER:O	2.15	0.47
1:A:2344:U:H2'	1:A:2345:A:C8	2.50	0.47
1:A:2427:U:H3	1:A:2602:G:H1	1.63	0.47
46:W:214:ARG:HH22	46:W:256:LYS:HE2	1.80	0.47
3:C:9:A:H2'	3:C:10:A:C8	2.49	0.46
1:A:597:G:H2'	1:A:598:A:C8	2.49	0.46
1:A:914:A:C5	5:LD:199:THR:HG21	2.49	0.46
1:A:2196:C:H2'	1:A:2242:A:H61	1.80	0.46
1:A:2266:U:H2'	1:A:2267:C:C6	2.50	0.46
5:LD:51:ASP:HB3	5:LD:54:ARG:HB3	1.97	0.46
8:LG:103:LEU:O	8:LG:107:ARG:HG2	2.15	0.46
17:LP:141:ALA:O	17:LP:145:ASP:HB2	2.15	0.46
40:Lm:66:ILE:HD12	40:Lm:66:ILE:H	1.80	0.46
47:V:253:LYS:HD3	47:V:254:ASP:OD1	2.16	0.46
14:LM:19:LEU:O	14:LM:68:HIS:HA	2.16	0.46
15:LN:182:ILE:HD12	15:LN:182:ILE:HA	1.82	0.46
33:Lf:15:ASN:OD1	33:Lf:18:LYS:HG3	2.16	0.46
47:V:90:LYS:NZ	47:V:94:LYS:HB3	2.30	0.46
30:Lc:41:HIS:O	30:Lc:45:MET:HB2	2.16	0.46
32:Le:14:LEU:O	32:Le:18:ILE:HG12	2.15	0.46
32:Le:16:LEU:HA	32:Le:19:LYS:HG2	1.96	0.46
45:X:97:VAL:HG13	45:X:99:GLU:HG2	1.97	0.46
28:La:89:LYS:HB3	28:La:89:LYS:HE3	1.83	0.46
30:Lc:72:VAL:HG13	30:Lc:113:LEU:HD23	1.97	0.46
38:Lk:94:ILE:HG22	38:Lk:98:ARG:HH11	1.80	0.46
1:A:159:A:H2'	1:A:160:G:H8	1.80	0.46
1:A:3306:U:H2'	1:A:3307:A:H5''	1.97	0.46
19:LR:37:ASN:HD22	19:LR:38:GLY:N	2.13	0.46
47:V:47:GLN:HE22	47:V:51:ARG:HH21	1.64	0.46
1:A:629:U:H2'	1:A:630:A:C8	2.51	0.46
1:A:650:C:H2'	1:A:651:G:C8	2.51	0.46
1:A:791:A:H2'	1:A:792:G:H8	1.81	0.46
10:LI:121:LYS:HA	10:LI:121:LYS:HD2	1.76	0.46
29:Lb:48:ARG:HB3	29:Lb:69:LYS:HB3	1.98	0.46
30:Lc:77:LYS:O	30:Lc:80:THR:HG22	2.16	0.46
33:Lf:20:LEU:HD11	33:Lf:32:ALA:HB2	1.98	0.46
1:A:1378:U:H2'	1:A:1379:G:H8	1.80	0.46
1:A:1596:C:H2'	1:A:1597:C:C6	2.51	0.46
1:A:2129:U:H2'	1:A:2130:G:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:LD:126:LEU:HD13	5:LD:150:LEU:HD21	1.97	0.46
14:LM:40:LEU:HD13	14:LM:125:MET:HE1	1.97	0.46
1:A:19:U:H2'	1:A:20:A:C8	2.51	0.46
1:A:3260:G:H5''	16:LO:125:LYS:HB3	1.97	0.46
4:z:398:MET:O	4:z:402:GLN:HG2	2.16	0.46
6:LE:53:MET:HG3	6:LE:77:THR:HG22	1.97	0.46
11:LJ:143:ILE:HG23	11:LJ:175:VAL:HG11	1.97	0.46
18:LQ:85:ARG:HG3	18:LQ:99:LEU:HD11	1.98	0.46
45:X:199:VAL:HG11	45:X:222:PHE:CZ	2.51	0.46
46:W:185:ILE:HG12	46:W:189:LYS:HZ2	1.81	0.46
47:V:171:PHE:O	47:V:175:GLU:HG2	2.16	0.46
47:V:179:LEU:HD11	47:V:415:LYS:HB2	1.98	0.46
1:A:985:U:H2'	1:A:986:U:H6	1.80	0.46
1:A:1108:U:H2'	1:A:1109:U:C6	2.51	0.46
1:A:2819:A:N6	1:A:2870:C:O2	2.49	0.46
12:LK:124:ARG:H	12:LK:124:ARG:HG2	1.59	0.46
6:LE:284:ARG:HH22	6:LE:296:THR:HG22	1.81	0.45
6:LE:372:THR:HG22	6:LE:374:ALA:H	1.81	0.45
1:A:243:G:H2'	1:A:244:G:O4'	2.16	0.45
1:A:314:U:H2'	1:A:315:C:C6	2.52	0.45
1:A:656:A:H2'	1:A:657:A:H8	1.81	0.45
1:A:946:U:H2'	1:A:947:G:H8	1.81	0.45
2:B:94:C:H2'	2:B:95:A:H8	1.82	0.45
6:LE:21:ARG:HB3	6:LE:272:TYR:HD2	1.81	0.45
42:Lo:99:CYS:HB2	42:Lo:114:LYS:HE3	1.97	0.45
1:A:1083:G:H2'	1:A:1084:A:H8	1.81	0.45
1:A:2423:U:H2'	1:A:2424:A:H8	1.82	0.45
5:LD:134:VAL:HG22	5:LD:151:PRO:HD3	1.98	0.45
19:LR:19:GLY:HA3	19:LR:22:LEU:HD11	1.98	0.45
26:LY:6:ASP:OD1	26:LY:13:ILE:HD11	2.16	0.45
45:X:151:TYR:OH	45:X:192:PHE:CE2	2.69	0.45
1:A:589:A:H1'	1:A:1337:A:H5''	1.99	0.45
1:A:1194:G:H2'	1:A:1195:A:C8	2.52	0.45
9:LH:11:PRO:HG2	34:Lg:91:THR:HG21	1.98	0.45
15:LN:62:THR:HG21	30:Lc:66:ALA:HB1	1.99	0.45
17:LP:33:LYS:HB3	17:LP:37:HIS:HD1	1.81	0.45
1:A:627:U:H2'	1:A:628:A:C8	2.51	0.45
1:A:2154:U:H2'	1:A:2155:G:H8	1.81	0.45
2:B:28:C:H1'	2:B:55:A:H61	1.82	0.45
5:LD:46:LYS:HA	5:LD:46:LYS:HD2	1.74	0.45
5:LD:60:LYS:HD2	5:LD:75:ILE:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:LI:184:LEU:HD21	10:LI:202:LEU:HD21	1.98	0.45
19:LR:60:PHE:HB3	19:LR:64:ASN:HB3	1.99	0.45
20:LS:40:THR:HG22	20:LS:42:ALA:H	1.82	0.45
38:Lk:36:ARG:O	38:Lk:40:VAL:HG23	2.17	0.45
46:W:208:ARG:NH2	46:W:494:GLY:HA2	2.32	0.45
1:A:2632:G:H5''	23:LV:12:ARG:HB2	1.97	0.45
1:A:2697:A:H2'	1:A:2698:G:H8	1.81	0.45
1:A:2836:C:H5	1:A:2852:C:H42	1.64	0.45
13:LL:30:LYS:HE3	13:LL:30:LYS:HB3	1.67	0.45
35:Lh:60:ARG:HD3	35:Lh:60:ARG:HA	1.80	0.45
1:A:215:G:H5''	28:La:12:ARG:HG3	1.98	0.45
1:A:824:C:H5''	5:LD:21:ARG:HD3	1.98	0.45
8:LG:105:ILE:O	8:LG:109:THR:HG23	2.17	0.45
13:LL:30:LYS:HG3	13:LL:63:GLU:HG3	1.98	0.45
19:LR:16:SER:HB3	19:LR:149:VAL:HG22	1.98	0.45
1:A:307:A:H2'	1:A:308:A:H8	1.82	0.45
1:A:3064:U:H2'	1:A:3065:G:H8	1.82	0.45
1:A:3107:U:H2'	1:A:3108:G:H8	1.82	0.45
3:C:131:A:H2'	3:C:132:G:H8	1.82	0.45
4:z:401:MET:HE1	41:Ln:23:LEU:HD12	1.99	0.45
6:LE:44:THR:OG1	6:LE:182:GLN:HB3	2.17	0.45
17:LP:140:LYS:HD3	17:LP:143:ARG:HD2	1.98	0.45
46:W:338:ASN:HA	46:W:384:MET:O	2.16	0.45
1:A:169:U:H4'	15:LN:128:ARG:HH21	1.82	0.45
7:LF:323:VAL:HG23	7:LF:326:ARG:HD2	1.98	0.45
11:LJ:140:VAL:HG22	11:LJ:166:LEU:HD21	1.99	0.45
13:LL:52:LEU:HB2	13:LL:152:LEU:HD13	1.98	0.45
16:LO:36:VAL:HG11	16:LO:55:ARG:HH22	1.81	0.45
26:LY:35:LYS:HE3	26:LY:51:TRP:CZ2	2.52	0.45
33:Lf:77:ARG:HD2	33:Lf:89:LEU:HD13	1.98	0.45
1:A:612:U:H2'	1:A:613:G:H8	1.82	0.45
1:A:656:A:H2'	1:A:657:A:C8	2.51	0.45
1:A:3162:C:H2'	1:A:3163:A:C8	2.52	0.45
9:LH:43:LEU:HG	35:Lh:102:LEU:HB2	1.99	0.45
9:LH:85:ILE:HG23	35:Lh:107:ILE:HB	1.98	0.45
17:LP:35:VAL:O	17:LP:64:VAL:HA	2.16	0.45
23:LV:85:LEU:HD23	23:LV:85:LEU:HA	1.85	0.45
28:La:23:PRO:O	28:La:27:ARG:HG3	2.17	0.45
38:Lk:5:THR:HG23	38:Lk:12:ASN:HB2	1.99	0.45
46:W:317:PHE:HE1	46:W:356:LEU:HD23	1.81	0.45
47:V:51:ARG:HA	47:V:134:VAL:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:U:H2'	1:A:139:G:H8	1.83	0.44
1:A:267:G:H4'	17:LP:50:ARG:HE	1.82	0.44
1:A:840:C:H2'	1:A:841:A:H8	1.82	0.44
1:A:1689:U:H5''	21:LT:61:SER:HB2	2.00	0.44
1:A:2218:G:H2'	1:A:2219:A:H8	1.82	0.44
28:La:122:LYS:HE3	28:La:122:LYS:HB3	1.75	0.44
1:A:541:U:H2'	1:A:542:G:C8	2.52	0.44
1:A:780:A:N6	20:LS:173:GLU:HB3	2.32	0.44
1:A:2103:U:H2'	1:A:2104:A:C8	2.52	0.44
1:A:2197:C:H4'	1:A:2198:A:H5'	1.98	0.44
1:A:2918:G:H2'	1:A:2919:A:H8	1.81	0.44
2:B:14:U:H5''	8:LG:24:ARG:HD3	1.99	0.44
12:LK:87:LYS:HE3	12:LK:187:ILE:HG12	1.97	0.44
22:LU:15:PRO:HB3	22:LU:22:PRO:HD3	1.99	0.44
37:Lj:73:LYS:H	37:Lj:73:LYS:HG2	1.58	0.44
40:Lm:14:LEU:HD21	40:Lm:52:TYR:CG	2.52	0.44
43:Lq:23:HIS:CD2	43:Lq:72:LEU:HB3	2.53	0.44
47:V:52:GLU:HA	47:V:135:GLU:O	2.17	0.44
47:V:320:VAL:HA	47:V:340:VAL:HG23	1.99	0.44
1:A:754:G:H2'	1:A:755:A:H8	1.82	0.44
1:A:3015:G:H2'	1:A:3016:A:C8	2.51	0.44
6:LE:47:LEU:HD22	6:LE:335:ILE:HD11	1.98	0.44
18:LQ:12:LYS:HD2	18:LQ:40:GLU:HG2	1.98	0.44
47:V:165:VAL:HG11	47:V:252:CYS:SG	2.57	0.44
1:A:129:U:H2'	1:A:130:A:C8	2.53	0.44
1:A:2183:A:H5''	5:LD:7:ASN:HD22	1.82	0.44
2:B:112:G:H2'	2:B:113:C:C6	2.52	0.44
7:LF:317:PRO:HA	7:LF:323:VAL:HG13	1.99	0.44
15:LN:85:LEU:HD13	15:LN:120:GLN:HE22	1.82	0.44
16:LO:74:ARG:HH11	16:LO:74:ARG:HG2	1.83	0.44
20:LS:60:PRO:HB2	20:LS:142:GLY:HA3	1.99	0.44
22:LU:27:MET:HE1	22:LU:44:PHE:CD2	2.53	0.44
28:La:102:SER:HB2	28:La:103:LYS:HE2	1.98	0.44
1:A:846:A:H2'	1:A:847:A:C8	2.51	0.44
1:A:1362:G:H2'	1:A:1363:A:C8	2.52	0.44
1:A:2931:C:H5''	25:LX:40:LYS:HE2	2.00	0.44
1:A:3164:C:O2'	1:A:3165:A:H8	2.00	0.44
6:LE:168:LYS:HB3	6:LE:319:ASN:HD21	1.81	0.44
12:LK:150:SER:HB3	12:LK:153:ASP:HB2	1.99	0.44
1:A:2241:U:H4'	5:LD:242:ARG:HB2	1.98	0.44
22:LU:74:ASN:HD21	22:LU:144:LEU:HD11	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2767:U:H2'	1:A:2768:U:C6	2.52	0.44
28:La:31:LEU:HB3	28:La:101:PRO:HG2	1.98	0.44
45:X:192:PHE:N	45:X:192:PHE:HD2	2.16	0.44
47:V:45:ILE:HG12	47:V:46:THR:HG23	2.00	0.44
47:V:103:ILE:HG22	47:V:113:ARG:HG3	2.00	0.44
1:A:616:G:H2'	1:A:617:G:C8	2.53	0.44
1:A:1666:G:H2'	1:A:1667:A:C8	2.52	0.44
1:A:2948:C:H5''	6:LE:243:HIS:HB3	2.00	0.44
7:LF:129:THR:HG21	7:LF:248:VAL:HB	2.00	0.44
9:LH:170:LYS:HB3	9:LH:172:HIS:CE1	2.53	0.44
32:Le:52:ARG:HE	32:Le:52:ARG:HB2	1.59	0.44
46:W:192:TRP:HA	46:W:195:VAL:HG12	1.99	0.44
47:V:219:PRO:HD3	47:V:280:SER:O	2.18	0.44
1:A:1290:A:H2'	1:A:1291:A:C8	2.53	0.44
6:LE:112:ASP:O	6:LE:116:ARG:HG3	2.18	0.44
7:LF:57:GLY:HA3	7:LF:98:ARG:HB2	2.00	0.44
25:LX:132:ASN:ND2	45:X:192:PHE:CZ	2.79	0.44
26:LY:17:ARG:HD2	26:LY:17:ARG:HA	1.66	0.44
27:LZ:131:ASP:HB3	27:LZ:134:ASP:HB3	1.99	0.44
41:Ln:28:ARG:HA	41:Ln:33:ASN:ND2	2.33	0.44
45:X:107:VAL:HG23	45:X:108:ILE:HG13	2.00	0.44
1:A:546:C:H4'	1:A:547:G:C4	2.53	0.43
1:A:1281:G:H2'	1:A:1282:G:H8	1.83	0.43
1:A:1369:A:H5''	30:Lc:21:ARG:HH11	1.83	0.43
1:A:2152:A:H2'	1:A:2153:U:H6	1.83	0.43
2:B:4:U:H2'	2:B:5:G:H8	1.82	0.43
6:LE:17:LEU:HD11	6:LE:233:TRP:HH2	1.82	0.43
10:LI:35:ALA:O	10:LI:39:GLU:HG3	2.18	0.43
16:LO:20:VAL:HG12	16:LO:32:LEU:HD22	2.00	0.43
19:LR:69:ARG:HB3	19:LR:79:THR:HG22	1.98	0.43
43:Lq:9:LYS:HE2	43:Lq:9:LYS:HB3	1.88	0.43
45:X:111:ASN:HB3	45:X:154:LEU:HG	2.00	0.43
45:X:218:ILE:O	45:X:222:PHE:HB2	2.18	0.43
1:A:1110:U:H2'	1:A:1111:U:C6	2.53	0.43
1:A:2154:U:H2'	1:A:2155:G:C8	2.53	0.43
5:LD:190:ARG:HH11	5:LD:190:ARG:HG2	1.82	0.43
11:LJ:64:ILE:O	11:LJ:68:ARG:HG2	2.18	0.43
13:LL:200:LEU:HD12	13:LL:213:PHE:HD2	1.82	0.43
23:LV:17:ARG:HE	23:LV:47:SER:HB3	1.83	0.43
44:Lr:85:ARG:HE	44:Lr:85:ARG:HB3	1.61	0.43
45:X:186:VAL:O	45:X:190:SER:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:A:H2'	1:A:274:G:H8	1.83	0.43
1:A:501:A:H2'	1:A:502:U:C6	2.54	0.43
1:A:1061:A:H4'	23:LV:102:ARG:HH21	1.83	0.43
1:A:2213:A:H2'	1:A:2214:A:C8	2.54	0.43
2:B:84:A:H2'	2:B:85:G:C8	2.53	0.43
3:C:63:G:H22	3:C:97:A:H2	1.66	0.43
12:LK:121:LYS:HA	12:LK:121:LYS:HD2	1.86	0.43
20:LS:67:ILE:HG23	20:LS:81:VAL:HG11	1.99	0.43
21:LT:43:LYS:HB2	21:LT:43:LYS:HE2	1.75	0.43
22:LU:13:ARG:HD3	22:LU:51:VAL:HB	2.00	0.43
34:Lg:86:THR:HG22	34:Lg:115:LEU:HD13	2.00	0.43
37:Lj:19:SER:HA	37:Lj:22:VAL:HG12	2.01	0.43
46:W:344:TYR:CE2	46:W:392:VAL:HG23	2.53	0.43
1:A:1119:C:H2'	1:A:1120:A:C8	2.53	0.43
1:A:1342:C:H2'	1:A:1343:A:H8	1.84	0.43
1:A:1783:U:H2'	1:A:1784:G:C8	2.54	0.43
1:A:1909:A:H2'	1:A:1910:A:C8	2.53	0.43
11:LJ:86:THR:O	11:LJ:90:THR:HG22	2.18	0.43
32:Le:25:LEU:HB3	32:Le:87:VAL:HG13	2.00	0.43
42:Lo:103:LEU:HD11	42:Lo:110:CYS:HA	2.00	0.43
43:Lq:29:LYS:HE3	43:Lq:29:LYS:HA	2.00	0.43
45:X:26:VAL:HG13	45:X:34:PHE:HE1	1.82	0.43
1:A:1104:G:H2'	1:A:1105:A:H8	1.84	0.43
1:A:2228:A:H2'	1:A:2229:A:H8	1.83	0.43
4:z:414:ARG:HE	19:LR:126:ARG:NH1	2.16	0.43
14:LM:16:LYS:HB2	14:LM:70:THR:HG23	2.00	0.43
17:LP:140:LYS:HA	17:LP:143:ARG:HB3	2.00	0.43
19:LR:129:THR:HG23	19:LR:131:ARG:HD3	2.01	0.43
46:W:465:ALA:HB1	46:W:470:TYR:HB2	2.00	0.43
2:B:59:U:H2'	2:B:60:G:H8	1.83	0.43
6:LE:188:ILE:O	6:LE:192:VAL:HG22	2.18	0.43
18:LQ:19:LEU:HD23	18:LQ:41:LEU:HD11	2.00	0.43
24:LW:93:ILE:HA	24:LW:106:ALA:O	2.19	0.43
1:A:664:U:H2'	1:A:665:A:H8	1.84	0.43
1:A:1054:A:H5''	1:A:2637:A:H61	1.84	0.43
1:A:1322:U:H2'	1:A:1323:G:H8	1.84	0.43
1:A:2882:U:H2'	1:A:2883:U:C6	2.53	0.43
1:A:3359:A:H2'	1:A:3360:C:C6	2.53	0.43
5:LD:54:ARG:HG2	5:LD:56:ALA:H	1.84	0.43
7:LF:233:LEU:HD23	7:LF:233:LEU:HA	1.83	0.43
47:V:159:VAL:HG12	47:V:244:TYR:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2351:U:H2'	1:A:2352:A:C8	2.51	0.43
1:A:2680:A:C4	14:LM:57:PHE:HE2	2.36	0.43
1:A:2880:U:H1'	6:LE:250:ALA:HB3	2.00	0.43
1:A:3033:A:H2'	1:A:3034:C:H6	1.83	0.43
6:LE:74:GLU:OE2	6:LE:325:LYS:HE2	2.19	0.43
9:LH:60:ASP:OD2	9:LH:62:THR:HG22	2.19	0.43
10:LI:180:SER:H	10:LI:183:ASP:HB2	1.84	0.43
15:LN:119:TYR:O	15:LN:123:ILE:HG23	2.18	0.43
47:V:85:CYS:HA	47:V:88:ARG:HD3	1.99	0.43
1:A:631:U:H2'	1:A:632:G:C8	2.53	0.43
1:A:2095:G:H2'	1:A:2096:A:C8	2.54	0.43
1:A:2222:A:H2'	1:A:2223:A:C8	2.54	0.43
2:B:4:U:H2'	2:B:5:G:C8	2.53	0.43
8:LG:107:ARG:HG3	8:LG:247:ILE:HG22	2.01	0.43
12:LK:38:LEU:HD13	12:LK:71:VAL:HG13	2.01	0.43
17:LP:106:VAL:HG21	17:LP:132:VAL:HG21	2.01	0.43
20:LS:178:ARG:HD2	20:LS:178:ARG:HA	1.72	0.43
1:A:1660:C:H2'	1:A:1661:G:C8	2.54	0.43
1:A:3001:C:H4'	6:LE:117:ARG:HG3	2.00	0.43
1:A:3322:A:H2'	1:A:3323:A:H8	1.83	0.43
8:LG:41:LYS:HA	8:LG:41:LYS:HD2	1.79	0.43
8:LG:178:ASN:HA	8:LG:183:TRP:CG	2.54	0.43
14:LM:60:ARG:HG2	14:LM:61:ARG:H	1.84	0.43
21:LT:21:LYS:HA	21:LT:21:LYS:HD3	1.74	0.43
25:LX:57:MET:HA	25:LX:76:ALA:O	2.19	0.43
25:LX:103:ALA:HA	25:LX:109:MET:HA	2.00	0.43
41:Ln:5:LYS:HE2	41:Ln:13:MET:HE1	2.00	0.43
1:A:900:G:H1'	1:A:1589:A:N6	2.34	0.42
1:A:2611:U:H2'	1:A:2612:U:C6	2.53	0.42
1:A:2844:C:H42	1:A:2898:G:H22	1.67	0.42
1:A:3280:U:HO2'	1:A:3281:U:H6	1.66	0.42
8:LG:289:LYS:HD2	13:LL:206:LEU:HD22	2.01	0.42
15:LN:62:THR:HG22	15:LN:64:LYS:H	1.84	0.42
39:Ll:8:PHE:O	39:Ll:11:ARG:HG2	2.19	0.42
46:W:168:HIS:O	46:W:172:SER:HB3	2.19	0.42
46:W:417:TYR:CD2	46:W:481:PRO:HB3	2.54	0.42
47:V:55:ILE:HD11	47:V:136:TYR:CD1	2.42	0.42
12:LK:4:ILE:HD11	22:LU:148:LEU:HD11	2.01	0.42
12:LK:99:ILE:HG22	12:LK:117:PHE:HA	2.00	0.42
20:LS:76:ALA:HA	20:LS:79:LYS:HD2	2.01	0.42
27:LZ:91:ASN:OD1	27:LZ:94:GLN:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Lc:81:LEU:HD21	30:Lc:109:TYR:HE1	1.84	0.42
38:Lk:61:ILE:HD13	38:Lk:61:ILE:HA	1.95	0.42
45:X:61:ARG:HD3	45:X:106:ASN:OD1	2.18	0.42
47:V:383:LEU:HD12	47:V:383:LEU:H	1.83	0.42
1:A:21:G:H3'	1:A:22:G:H8	1.83	0.42
1:A:312:C:H2'	1:A:313:A:C8	2.54	0.42
1:A:848:A:C5	1:A:849:C:H1'	2.54	0.42
1:A:993:G:N3	1:A:2637:A:H2'	2.33	0.42
1:A:1060:U:H2'	1:A:1061:A:C8	2.54	0.42
1:A:3138:U:H2'	1:A:3139:A:H8	1.85	0.42
6:LE:332:ARG:HD3	6:LE:332:ARG:H	1.84	0.42
15:LN:128:ARG:HH11	15:LN:128:ARG:HB2	1.84	0.42
34:Lg:54:LYS:HB3	34:Lg:54:LYS:HE2	1.67	0.42
37:Lj:94:LYS:HB3	37:Lj:94:LYS:HE2	1.87	0.42
45:X:192:PHE:N	45:X:192:PHE:CD2	2.87	0.42
1:A:903:U:H2'	1:A:904:A:C8	2.54	0.42
1:A:2366:C:H2'	1:A:2367:A:H8	1.85	0.42
1:A:2368:A:H2'	1:A:2369:G:C8	2.55	0.42
1:A:2914:G:H5''	6:LE:9:PRO:HG3	2.00	0.42
1:A:3160:U:O4	1:A:3290:G:O6	2.37	0.42
3:C:67:U:H2'	3:C:68:G:H8	1.84	0.42
8:LG:151:GLN:OE1	8:LG:159:VAL:HG11	2.19	0.42
47:V:178:ILE:HG22	47:V:184:HIS:ND1	2.35	0.42
47:V:413:LYS:HG2	47:V:468:ASN:HB3	2.00	0.42
1:A:20:A:H2'	1:A:21:G:C8	2.54	0.42
1:A:624:G:H2'	1:A:625:G:H8	1.85	0.42
1:A:1667:A:H2'	1:A:1668:G:C8	2.54	0.42
1:A:2261:G:H2'	46:W:375:GLN:HE22	1.84	0.42
1:A:2368:A:H2'	1:A:2369:G:H8	1.85	0.42
1:A:2423:U:H2'	1:A:2424:A:C8	2.53	0.42
1:A:2428:U:H2'	1:A:2429:G:H8	1.84	0.42
1:A:2970:C:H2'	1:A:2972:G:C8	2.54	0.42
1:A:3281:U:H2'	1:A:3282:U:C6	2.55	0.42
2:B:79:A:H62	2:B:101:G:H21	1.68	0.42
5:LD:150:LEU:HD23	5:LD:150:LEU:HA	1.85	0.42
5:LD:238:ILE:HD13	5:LD:238:ILE:HA	1.81	0.42
7:LF:205:PRO:HG2	7:LF:225:VAL:HG13	2.01	0.42
17:LP:178:HIS:CE1	17:LP:179:LYS:HG3	2.53	0.42
18:LQ:171:LYS:O	18:LQ:175:THR:HG22	2.19	0.42
20:LS:110:ALA:O	20:LS:114:ILE:HD12	2.20	0.42
22:LU:93:GLU:HG2	22:LU:137:ARG:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Lc:63:LYS:HD2	30:Lc:68:PHE:HE2	1.84	0.42
47:V:412:TRP:NE1	47:V:491:ILE:HG13	2.34	0.42
1:A:928:C:H2'	1:A:929:A:C8	2.54	0.42
1:A:1307:G:H1'	1:A:1308:A:C8	2.54	0.42
1:A:2436:U:H2'	1:A:2437:G:H5''	2.01	0.42
1:A:3110:C:H2'	1:A:3111:U:C6	2.54	0.42
6:LE:117:ARG:HA	6:LE:175:LYS:HE3	2.02	0.42
10:LI:178:ILE:HG23	10:LI:183:ASP:HB3	2.00	0.42
15:LN:159:VAL:HG21	30:Lc:96:LYS:HE3	2.02	0.42
20:LS:24:VAL:HA	20:LS:27:LYS:HE3	2.02	0.42
27:LZ:86:VAL:HG11	27:LZ:95:ILE:HD11	2.01	0.42
32:Le:16:LEU:HD22	32:Le:98:SER:HB2	2.01	0.42
45:X:66:ASN:HD21	45:X:133:LEU:HB3	1.83	0.42
45:X:157:GLN:HE22	45:X:201:ASP:HA	1.84	0.42
1:A:155:G:H5''	1:A:156:G:H2'	2.02	0.42
1:A:1114:U:H5''	30:Lc:22:ILE:HD13	2.01	0.42
1:A:1896:A:H61	1:A:2339:C:H42	1.68	0.42
8:LG:22:ARG:HH21	8:LG:27:LYS:HD2	1.84	0.42
22:LU:45:LEU:HD12	22:LU:45:LEU:HA	1.84	0.42
22:LU:101:ALA:O	22:LU:105:THR:HG22	2.20	0.42
24:LW:84:LEU:HD13	24:LW:93:ILE:HG13	2.01	0.42
1:A:1349:G:H2'	1:A:1350:A:O4'	2.20	0.42
1:A:1460:A:H2'	1:A:1461:A:H8	1.84	0.42
1:A:1650:G:H5'	5:LD:70:ARG:HG2	2.02	0.42
2:B:94:C:H2'	2:B:95:A:C8	2.55	0.42
6:LE:283:TYR:CZ	6:LE:325:LYS:HG3	2.54	0.42
11:LJ:81:THR:HG22	11:LJ:179:ILE:HG22	2.02	0.42
13:LL:174:THR:HG22	13:LL:196:PHE:HE1	1.85	0.42
43:Lq:22:GLN:HE21	43:Lq:22:GLN:HB2	1.60	0.42
1:A:1696:A:H2'	1:A:1697:A:C8	2.55	0.42
1:A:2217:U:H2'	1:A:2218:G:H8	1.85	0.42
6:LE:41:VAL:HA	6:LE:185:GLY:HA3	2.01	0.42
13:LL:49:CYS:HA	13:LL:138:VAL:O	2.19	0.42
20:LS:126:GLN:HA	20:LS:129:VAL:HG12	2.02	0.42
30:Lc:132:LYS:HG2	30:Lc:136:GLU:OE2	2.19	0.42
32:Le:18:ILE:HD11	32:Le:81:VAL:HG12	2.01	0.42
35:Lh:20:LYS:HG2	35:Lh:21:ARG:HD3	2.01	0.42
39:LI:64:MET:O	39:LI:68:LYS:HD2	2.19	0.42
1:A:531:G:H2'	1:A:532:A:C8	2.55	0.42
1:A:563:U:H2'	1:A:564:G:H8	1.84	0.42
1:A:1660:C:H2'	1:A:1661:G:H8	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1663:C:H2'	1:A:1664:G:H8	1.84	0.42
1:A:1709:C:H2'	1:A:1710:C:H6	1.85	0.42
1:A:2407:C:H2'	1:A:2408:U:H6	1.85	0.42
9:LH:70:LYS:HE3	9:LH:70:LYS:HB3	1.74	0.42
10:LI:37:ASN:O	10:LI:41:ARG:HG2	2.20	0.42
45:X:71:LEU:HD23	45:X:71:LEU:HA	1.83	0.42
1:A:68:C:O3'	17:LP:177:GLY:HA2	2.20	0.41
1:A:1680:G:H2'	1:A:1681:U:H6	1.85	0.41
1:A:1785:U:H2'	1:A:1786:G:C8	2.55	0.41
1:A:1881:A:H2'	1:A:1882:G:H8	1.84	0.41
14:LM:37:LEU:HD12	14:LM:67:VAL:HG12	2.03	0.41
34:Lg:101:SER:O	34:Lg:105:ARG:HG3	2.19	0.41
38:Lk:85:ALA:O	38:Lk:88:GLU:HG3	2.20	0.41
1:A:207:U:H2'	1:A:208:C:C6	2.55	0.41
1:A:597:G:H5''	10:LI:41:ARG:NH1	2.35	0.41
1:A:2545:C:H2'	1:A:2546:C:C6	2.55	0.41
14:LM:32:ARG:O	14:LM:36:VAL:HG23	2.19	0.41
15:LN:67:ARG:H	15:LN:67:ARG:HG2	1.61	0.41
47:V:65:LEU:HD11	47:V:69:GLY:HA2	2.01	0.41
1:A:29:C:H4'	1:A:62:A:H4'	2.01	0.41
5:LD:33:ASP:O	5:LD:37:ARG:HG2	2.20	0.41
7:LF:154:THR:O	7:LF:157:GLU:HG3	2.20	0.41
14:LM:160:VAL:O	14:LM:164:LYS:HG2	2.20	0.41
34:Lg:104:ASN:O	34:Lg:108:ILE:HG13	2.20	0.41
1:A:2242:A:H5''	5:LD:244:GLY:HA3	2.02	0.41
5:LD:47:GLN:HG3	5:LD:49:VAL:HG13	2.03	0.41
13:LL:166:ILE:HD11	23:LV:158:THR:HG21	2.02	0.41
14:LM:81:GLU:HG2	14:LM:167:TYR:HE2	1.86	0.41
16:LO:17:VAL:HG21	16:LO:74:ARG:HB2	2.02	0.41
18:LQ:7:VAL:HG23	18:LQ:31:GLN:HE22	1.85	0.41
32:Le:56:LEU:HD13	32:Le:56:LEU:HA	1.96	0.41
1:A:286:U:H2'	1:A:287:G:C8	2.56	0.41
1:A:561:C:OP1	16:LO:77:ARG:HG3	2.21	0.41
1:A:840:C:H2'	1:A:841:A:C8	2.56	0.41
1:A:2260:U:H3'	1:A:2261:G:H5''	2.02	0.41
1:A:2401:A:H1'	4:z:432:GLN:HB3	2.01	0.41
1:A:2407:C:H2'	1:A:2408:U:C6	2.56	0.41
1:A:2419:A:H2'	1:A:2420:C:C6	2.55	0.41
1:A:2532:U:H2'	1:A:2533:G:C8	2.55	0.41
1:A:3293:U:H5'	6:LE:128:LYS:HZ1	1.85	0.41
5:LD:111:THR:HG22	5:LD:113:VAL:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:LE:298:PHE:CD1	6:LE:357:LYS:HG2	2.55	0.41
8:LG:190:ILE:HD11	8:LG:195:LEU:HD23	2.03	0.41
10:LI:224:ILE:HD12	22:LU:36:ILE:HA	2.03	0.41
13:LL:138:VAL:HG11	13:LL:148:VAL:HB	2.03	0.41
15:LN:4:SER:O	15:LN:5:LYS:HD3	2.21	0.41
19:LR:37:ASN:HD22	19:LR:37:ASN:C	2.29	0.41
26:LY:57:LYS:HB2	26:LY:57:LYS:HE2	1.78	0.41
29:Lb:51:LEU:HB2	29:Lb:65:ARG:HB3	2.02	0.41
37:Lj:44:ILE:HD13	37:Lj:44:ILE:HA	1.87	0.41
38:Lk:70:ARG:HG3	38:Lk:87:VAL:HG21	2.01	0.41
47:V:47:GLN:HE21	47:V:47:GLN:HA	1.86	0.41
47:V:210:MET:O	47:V:214:LEU:HD12	2.21	0.41
47:V:226:GLU:HA	47:V:242:PHE:HA	2.02	0.41
1:A:94:G:H2'	1:A:95:A:C8	2.55	0.41
1:A:153:U:H4'	1:A:158:G:H4'	2.01	0.41
1:A:595:G:H1	1:A:609:G:H5''	1.85	0.41
1:A:727:G:H4'	1:A:977:C:H5'	2.01	0.41
1:A:887:G:H2'	1:A:888:A:C8	2.55	0.41
1:A:1472:U:H2'	1:A:1473:G:H8	1.86	0.41
1:A:2947:G:N3	6:LE:250:ALA:HB1	2.35	0.41
5:LD:83:HIS:CD2	5:LD:86:GLN:HB2	2.55	0.41
17:LP:37:HIS:NE2	17:LP:63:ARG:HB3	2.35	0.41
32:Le:25:LEU:HD11	32:Le:83:LYS:HD2	2.01	0.41
38:Lk:94:ILE:HA	38:Lk:97:SER:HB2	2.03	0.41
46:W:127:GLN:OE1	46:W:396:PHE:HB3	2.20	0.41
1:A:149:U:P	17:LP:49:ARG:HH12	2.43	0.41
1:A:407:A:C2	3:C:17:A:H1'	2.56	0.41
1:A:507:U:H2'	1:A:508:U:C6	2.56	0.41
1:A:985:U:H2'	1:A:986:U:C6	2.56	0.41
1:A:1060:U:H2'	1:A:1061:A:H8	1.86	0.41
1:A:3166:C:H2'	1:A:3167:A:H8	1.85	0.41
1:A:3295:A:H2'	1:A:3296:A:C8	2.55	0.41
6:LE:47:LEU:HD11	6:LE:179:ALA:HB3	2.02	0.41
6:LE:106:TRP:HH2	6:LE:178:LEU:HD21	1.85	0.41
8:LG:109:THR:HA	8:LG:112:LYS:HG2	2.02	0.41
8:LG:156:GLY:HA2	8:LG:181:PRO:HB3	2.02	0.41
22:LU:8:GLN:O	22:LU:61:ILE:HA	2.21	0.41
37:Lj:73:LYS:HE2	37:Lj:73:LYS:HB3	1.84	0.41
40:Lm:43:PHE:HE2	40:Lm:66:ILE:HG13	1.86	0.41
43:Lq:25:VAL:HG22	43:Lq:72:LEU:HD23	2.02	0.41
1:A:255:A:H2'	1:A:256:G:H8	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:584:G:H2'	1:A:585:A:H8	1.85	0.41
1:A:2428:U:H2'	1:A:2429:G:C8	2.56	0.41
1:A:3294:A:H2'	1:A:3295:A:O4'	2.20	0.41
11:LJ:172:LYS:HE2	11:LJ:172:LYS:HB2	1.94	0.41
15:LN:58:VAL:HG21	15:LN:72:GLY:HA3	2.02	0.41
18:LQ:106:GLU:HG2	18:LQ:147:TRP:CZ2	2.56	0.41
18:LQ:128:ARG:HE	18:LQ:128:ARG:HB3	1.64	0.41
45:X:63:THR:HB	45:X:70:LEU:HD11	2.02	0.41
45:X:66:ASN:HD22	45:X:133:LEU:HD13	1.86	0.41
1:A:129:U:H2'	1:A:130:A:H8	1.86	0.41
1:A:201:A:H2'	1:A:202:G:H8	1.85	0.41
1:A:253:A:H2'	1:A:254:A:C8	2.55	0.41
1:A:417:A:H2'	1:A:418:A:C8	2.56	0.41
1:A:899:U:H2'	1:A:900:G:H8	1.85	0.41
1:A:982:C:H2'	1:A:983:A:C8	2.56	0.41
1:A:1039:U:H2'	1:A:1040:A:C8	2.56	0.41
1:A:1430:U:C4	30:Lc:9:ARG:HD2	2.55	0.41
1:A:2102:U:H2'	1:A:2103:U:C6	2.56	0.41
1:A:2186:U:C5	5:LD:200:ARG:HD3	2.55	0.41
1:A:2369:G:H2'	1:A:2370:G:C8	2.56	0.41
1:A:2552:C:H2'	32:Le:50:VAL:HG11	2.02	0.41
1:A:3051:U:H2'	1:A:3052:G:H8	1.86	0.41
1:A:3181:C:H2'	1:A:3182:G:C8	2.55	0.41
1:A:3193:C:H2'	1:A:3194:C:C6	2.55	0.41
2:B:74:C:H2'	2:B:75:G:C8	2.56	0.41
5:LD:188:LYS:HD3	5:LD:189:TYR:CE2	2.56	0.41
11:LJ:115:ALA:HA	11:LJ:118:GLU:OE1	2.21	0.41
14:LM:172:LEU:HD23	14:LM:172:LEU:HA	1.90	0.41
16:LO:8:LYS:HD3	16:LO:8:LYS:HA	1.80	0.41
16:LO:28:SER:HA	16:LO:31:LYS:HE2	2.03	0.41
17:LP:143:ARG:NH1	37:Lj:92:LEU:HD23	2.36	0.41
21:LT:105:LEU:HD22	21:LT:135:LYS:HG3	2.03	0.41
24:LW:94:ARG:HD2	24:LW:108:TYR:HE2	1.86	0.41
30:Lc:59:ARG:HH22	43:Lq:38:GLN:NE2	2.19	0.41
37:Lj:92:LEU:HD22	37:Lj:96:GLU:HB3	2.01	0.41
46:W:117:ASN:HD22	46:W:119:GLN:HG2	1.86	0.41
46:W:135:ILE:HG22	46:W:162:TRP:CD1	2.54	0.41
47:V:49:ILE:HD12	47:V:49:ILE:H	1.85	0.41
47:V:209:LYS:HB3	47:V:209:LYS:HE3	1.79	0.41
1:A:1009:A:H2'	1:A:1010:G:C8	2.56	0.41
1:A:2544:U:H2'	1:A:2545:C:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2683:U:H2'	1:A:2684:C:C6	2.56	0.41
1:A:3167:A:H2'	1:A:3168:A:H8	1.86	0.41
9:LH:54:TYR:CE1	9:LH:63:LEU:HB2	2.56	0.41
12:LK:20:ILE:HB	16:LO:7:VAL:HG13	2.03	0.41
14:LM:107:ASP:HA	14:LM:124:GLY:HA2	2.03	0.41
23:LV:111:ALA:O	23:LV:115:LYS:HG3	2.21	0.41
25:LX:85:TRP:O	25:LX:92:PHE:HA	2.21	0.41
31:Ld:47:LEU:HA	31:Ld:50:THR:HG22	2.03	0.41
42:Lo:93:LYS:HB2	42:Lo:124:LYS:HE3	2.02	0.41
1:A:209:A:H4'	1:A:211:A:N7	2.35	0.40
1:A:255:A:H2'	1:A:256:G:C8	2.56	0.40
1:A:1283:C:H2'	1:A:1284:C:C5	2.56	0.40
1:A:1340:G:H2'	1:A:1341:U:C6	2.56	0.40
1:A:2107:A:H2	1:A:3344:A:H8	1.68	0.40
1:A:2263:C:H2'	1:A:2264:U:H6	1.84	0.40
1:A:3023:U:H2'	1:A:3024:A:C8	2.55	0.40
1:A:3166:C:H2'	1:A:3167:A:C8	2.55	0.40
11:LJ:112:GLU:O	11:LJ:116:VAL:HG22	2.21	0.40
13:LL:12:GLN:HA	13:LL:59:GLN:NE2	2.37	0.40
22:LU:95:ARG:HE	22:LU:95:ARG:HB2	1.76	0.40
35:Lh:9:VAL:HG21	35:Lh:44:TYR:HE2	1.86	0.40
38:Lk:29:LYS:HE2	38:Lk:29:LYS:HA	2.03	0.40
44:Lr:84:ARG:O	44:Lr:88:GLU:HG2	2.20	0.40
1:A:1109:U:H2'	1:A:1110:U:C6	2.56	0.40
1:A:1525:G:H5'	1:A:1830:G:OP2	2.20	0.40
1:A:1682:U:C6	24:LW:85:LYS:HG2	2.56	0.40
10:LI:116:PHE:CZ	10:LI:144:ILE:HG12	2.57	0.40
12:LK:128:VAL:HA	12:LK:157:ASN:HD21	1.86	0.40
19:LR:35:ALA:HB2	19:LR:58:ILE:HG23	2.03	0.40
29:Lb:88:ASP:HB3	29:Lb:121:ARG:HH12	1.86	0.40
30:Lc:99:ALA:HB1	30:Lc:123:VAL:HA	2.04	0.40
37:Lj:101:THR:HG23	37:Lj:103:LYS:H	1.85	0.40
38:Lk:40:VAL:O	38:Lk:44:VAL:HG23	2.21	0.40
43:Lq:46:LYS:HD3	43:Lq:54:THR:HG21	2.03	0.40
45:X:129:ILE:HD12	45:X:133:LEU:HD12	2.03	0.40
1:A:612:U:H2'	1:A:613:G:C8	2.56	0.40
1:A:1168:U:H1'	10:LI:209:ASN:ND2	2.36	0.40
1:A:2266:U:H2'	1:A:2267:C:H6	1.86	0.40
1:A:2352:A:H5''	19:LR:83:TRP:O	2.21	0.40
1:A:2661:G:H2'	1:A:2662:G:H8	1.87	0.40
13:LL:178:ARG:HB2	13:LL:179:PRO:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:LR:31:GLU:OE1	19:LR:60:PHE:HA	2.21	0.40
20:LS:178:ARG:HD3	30:Lc:50:PRO:HG2	2.04	0.40
26:LY:20:LEU:HD21	26:LY:28:ILE:HD12	2.02	0.40
44:Lr:48:LYS:HB3	44:Lr:48:LYS:HE2	1.86	0.40
45:X:217:VAL:HG21	47:V:18:LEU:HD22	2.04	0.40
46:W:135:ILE:HD13	46:W:135:ILE:HA	1.99	0.40
47:V:260:PRO:HD2	47:V:263:LEU:HD23	2.02	0.40
47:V:273:PHE:CE2	47:V:374:ILE:HD13	2.56	0.40
1:A:157:A:N7	38:Lk:26:ILE:HG12	2.36	0.40
1:A:158:G:H2'	1:A:159:A:H8	1.87	0.40
1:A:175:C:H2'	1:A:176:G:C8	2.56	0.40
1:A:662:U:H2'	1:A:663:C:C6	2.57	0.40
1:A:1095:U:H3	23:LV:127:GLN:HG3	1.86	0.40
1:A:2103:U:H2'	1:A:2104:A:H8	1.85	0.40
1:A:2987:A:O2'	6:LE:259:HIS:HB3	2.22	0.40
1:A:3332:U:H2'	1:A:3333:G:O4'	2.22	0.40
26:LY:2:LYS:HE3	26:LY:2:LYS:HB2	1.79	0.40
47:V:338:ILE:HD12	47:V:357:SER:HB2	2.04	0.40
1:A:1063:G:C6	23:LV:109:VAL:HG22	2.57	0.40
1:A:1336:U:H2'	1:A:1337:A:C8	2.55	0.40
5:LD:108:PRO:HG2	44:Lr:86:LEU:HD21	2.03	0.40
9:LH:102:ASN:HB2	9:LH:104:GLU:OE2	2.21	0.40
13:LL:43:VAL:HA	13:LL:139:ARG:HH12	1.87	0.40
17:LP:66:VAL:HG23	17:LP:98:LEU:HD23	2.03	0.40
34:Lg:87:MET:HE2	34:Lg:87:MET:HB2	1.93	0.40
34:Lg:91:THR:HG22	34:Lg:92:TYR:CD2	2.57	0.40
35:Lh:52:VAL:HG22	35:Lh:66:VAL:HG22	2.02	0.40
46:W:244:LYS:HE3	46:W:244:LYS:HB3	1.80	0.40
46:W:354:ASN:OD1	46:W:362:VAL:HG12	2.22	0.40
46:W:384:MET:HE2	46:W:384:MET:HB2	1.88	0.40
46:W:404:VAL:HB	46:W:409:LEU:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	z	54/432 (12%)	54 (100%)	0	0	100	100
5	LD	244/254 (96%)	238 (98%)	6 (2%)	0	100	100
6	LE	384/387 (99%)	375 (98%)	9 (2%)	0	100	100
7	LF	359/362 (99%)	343 (96%)	16 (4%)	0	100	100
8	LG	284/297 (96%)	281 (99%)	3 (1%)	0	100	100
9	LH	152/176 (86%)	143 (94%)	9 (6%)	0	100	100
10	LI	220/244 (90%)	214 (97%)	6 (3%)	0	100	100
11	LJ	224/256 (88%)	220 (98%)	4 (2%)	0	100	100
12	LK	186/191 (97%)	176 (95%)	10 (5%)	0	100	100
13	LL	205/210 (98%)	192 (94%)	13 (6%)	0	100	100
14	LM	165/174 (95%)	158 (96%)	7 (4%)	0	100	100
15	LN	191/199 (96%)	186 (97%)	4 (2%)	1 (0%)	24	43
16	LO	134/138 (97%)	129 (96%)	5 (4%)	0	100	100
17	LP	201/204 (98%)	198 (98%)	3 (2%)	0	100	100
18	LQ	195/199 (98%)	194 (100%)	1 (0%)	0	100	100
19	LR	168/184 (91%)	159 (95%)	9 (5%)	0	100	100
20	LS	183/186 (98%)	175 (96%)	8 (4%)	0	100	100
21	LT	150/189 (79%)	148 (99%)	2 (1%)	0	100	100
22	LU	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
23	LV	157/160 (98%)	155 (99%)	2 (1%)	0	100	100
24	LW	96/121 (79%)	91 (95%)	5 (5%)	0	100	100
25	LX	134/137 (98%)	133 (99%)	1 (1%)	0	100	100
26	LY	60/155 (39%)	60 (100%)	0	0	100	100
27	LZ	118/142 (83%)	118 (100%)	0	0	100	100
28	La	123/127 (97%)	122 (99%)	1 (1%)	0	100	100
29	Lb	132/136 (97%)	131 (99%)	1 (1%)	0	100	100
30	Lc	146/149 (98%)	139 (95%)	7 (5%)	0	100	100
31	Ld	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
32	Le	94/105 (90%)	93 (99%)	1 (1%)	0	100	100
33	Lf	103/113 (91%)	103 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	Lg	124/130 (95%)	121 (98%)	3 (2%)	0	100	100
35	Lh	104/107 (97%)	101 (97%)	3 (3%)	0	100	100
36	Li	107/121 (88%)	106 (99%)	1 (1%)	0	100	100
37	Lj	117/120 (98%)	114 (97%)	3 (3%)	0	100	100
38	Lk	95/100 (95%)	93 (98%)	2 (2%)	0	100	100
39	Ll	79/88 (90%)	79 (100%)	0	0	100	100
40	Lm	74/78 (95%)	73 (99%)	1 (1%)	0	100	100
41	Ln	48/51 (94%)	48 (100%)	0	0	100	100
42	Lo	48/128 (38%)	48 (100%)	0	0	100	100
43	Lq	97/106 (92%)	91 (94%)	6 (6%)	0	100	100
44	Lr	89/92 (97%)	87 (98%)	2 (2%)	0	100	100
45	X	224/245 (91%)	207 (92%)	17 (8%)	0	100	100
46	W	287/640 (45%)	273 (95%)	14 (5%)	0	100	100
47	V	380/518 (73%)	358 (94%)	22 (6%)	0	100	100
All	All	6960/8382 (83%)	6745 (97%)	214 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	LN	47	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	z	51/392 (13%)	51 (100%)	0	100	100
5	LD	189/196 (96%)	187 (99%)	2 (1%)	65	81
6	LE	322/323 (100%)	315 (98%)	7 (2%)	45	69
7	LF	288/289 (100%)	286 (99%)	2 (1%)	76	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	LG	237/245 (97%)	234 (99%)	3 (1%)	61	79
9	LH	136/155 (88%)	132 (97%)	4 (3%)	37	61
10	LI	186/205 (91%)	184 (99%)	2 (1%)	65	81
11	LJ	187/208 (90%)	180 (96%)	7 (4%)	30	55
12	LK	168/171 (98%)	163 (97%)	5 (3%)	36	60
13	LL	177/179 (99%)	177 (100%)	0	100	100
14	LM	145/151 (96%)	138 (95%)	7 (5%)	23	46
15	LN	154/159 (97%)	148 (96%)	6 (4%)	28	53
16	LO	107/109 (98%)	105 (98%)	2 (2%)	50	73
17	LP	175/176 (99%)	171 (98%)	4 (2%)	44	68
18	LQ	160/162 (99%)	160 (100%)	0	100	100
19	LR	138/146 (94%)	137 (99%)	1 (1%)	76	88
20	LS	150/151 (99%)	147 (98%)	3 (2%)	48	72
21	LT	126/154 (82%)	123 (98%)	3 (2%)	43	67
22	LU	155/156 (99%)	153 (99%)	2 (1%)	61	79
23	LV	136/137 (99%)	135 (99%)	1 (1%)	76	88
24	LW	85/107 (79%)	82 (96%)	3 (4%)	32	57
25	LX	104/105 (99%)	101 (97%)	3 (3%)	37	61
26	LY	54/129 (42%)	51 (94%)	3 (6%)	19	40
27	LZ	104/118 (88%)	103 (99%)	1 (1%)	68	83
28	La	108/110 (98%)	106 (98%)	2 (2%)	50	73
29	Lb	115/116 (99%)	110 (96%)	5 (4%)	26	50
30	Lc	118/119 (99%)	115 (98%)	3 (2%)	42	66
31	Ld	46/47 (98%)	42 (91%)	4 (9%)	9	21
32	Le	81/88 (92%)	78 (96%)	3 (4%)	30	55
33	Lf	92/97 (95%)	90 (98%)	2 (2%)	45	69
34	Lg	108/111 (97%)	105 (97%)	3 (3%)	38	62
35	Lh	90/91 (99%)	88 (98%)	2 (2%)	45	69
36	Li	94/103 (91%)	93 (99%)	1 (1%)	65	81
37	Lj	104/105 (99%)	100 (96%)	4 (4%)	29	54
38	Lk	79/82 (96%)	78 (99%)	1 (1%)	61	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	Ll	67/71 (94%)	65 (97%)	2 (3%)	36	60
40	Lm	67/69 (97%)	65 (97%)	2 (3%)	36	60
41	Ln	45/46 (98%)	44 (98%)	1 (2%)	45	69
42	Lo	45/116 (39%)	45 (100%)	0	100	100
43	Lq	86/91 (94%)	84 (98%)	2 (2%)	44	68
44	Lr	71/72 (99%)	69 (97%)	2 (3%)	38	62
45	X	194/211 (92%)	192 (99%)	2 (1%)	68	83
46	W	257/555 (46%)	252 (98%)	5 (2%)	50	73
47	V	349/467 (75%)	336 (96%)	13 (4%)	30	55
All	All	5950/7090 (84%)	5820 (98%)	130 (2%)	45	69

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	LD	29	LEU
5	LD	191	LEU
6	LE	60	LEU
6	LE	90	VAL
6	LE	157	VAL
6	LE	300	ARG
6	LE	323	MET
6	LE	346	THR
6	LE	369	ARG
7	LF	54	GLU
7	LF	304	GLN
8	LG	84	PRO
8	LG	95	TRP
8	LG	208	MET
9	LH	65	VAL
9	LH	99	GLU
9	LH	145	LEU
9	LH	152	THR
10	LI	78	GLU
10	LI	233	GLU
11	LJ	36	ILE
11	LJ	74	THR
11	LJ	79	GLN
11	LJ	172	LYS
11	LJ	175	VAL

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Mol	Chain	Res	Type
11	LJ	203	VAL
11	LJ	246	MET
12	LK	12	VAL
12	LK	82	VAL
12	LK	140	VAL
12	LK	151	VAL
12	LK	162	GLN
14	LM	40	LEU
14	LM	46	VAL
14	LM	51	ARG
14	LM	59	ILE
14	LM	78	GLU
14	LM	79	ILE
14	LM	152	HIS
15	LN	3	ILE
15	LN	69	VAL
15	LN	134	GLU
15	LN	155	GLU
15	LN	164	GLU
15	LN	170	LEU
16	LO	12	TRP
16	LO	92	GLU
17	LP	61	ILE
17	LP	92	LEU
17	LP	104	GLU
17	LP	153	ASP
19	LR	79	THR
20	LS	31	LYS
20	LS	114	ILE
20	LS	165	ILE
21	LT	30	SER
21	LT	31	GLU
21	LT	53	LYS
22	LU	48	LEU
22	LU	172	TYR
23	LV	79	MET
24	LW	50	LEU
24	LW	64	THR
24	LW	65	VAL
25	LX	34	LEU
25	LX	96	GLU
25	LX	136	VAL

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Mol	Chain	Res	Type
26	LY	3	VAL
26	LY	6	ASP
26	LY	34	SER
27	LZ	133	LEU
28	La	11	ASP
28	La	120	GLN
29	Lb	6	LYS
29	Lb	24	VAL
29	Lb	89	VAL
29	Lb	128	GLN
29	Lb	134	LEU
30	Lc	89	GLN
30	Lc	147	LEU
30	Lc	148	ILE
31	Ld	14	ARG
31	Ld	23	LYS
31	Ld	47	LEU
31	Ld	48	HIS
32	Le	17	VAL
32	Le	52	ARG
32	Le	90	VAL
33	Lf	16	LEU
33	Lf	106	THR
34	Lg	95	GLU
34	Lg	109	LEU
34	Lg	126	LEU
35	Lh	74	THR
35	Lh	98	VAL
36	Li	107	GLU
37	Lj	28	LEU
37	Lj	38	ARG
37	Lj	44	ILE
37	Lj	51	ILE
38	Lk	34	SER
39	Ll	48	ASN
39	Ll	67	LEU
40	Lm	3	ARG
40	Lm	19	ASP
41	Ln	47	THR
43	Lq	21	THR
43	Lq	57	VAL
44	Lr	48	LYS

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Mol	Chain	Res	Type
44	Lr	89	MET
45	X	98	GLU
45	X	168	GLN
46	W	123	LEU
46	W	202	VAL
46	W	385	LEU
46	W	402	GLU
46	W	430	LYS
47	V	44	ASP
47	V	81	LEU
47	V	111	ARG
47	V	116	LEU
47	V	134	VAL
47	V	197	LEU
47	V	270	ILE
47	V	290	THR
47	V	320	VAL
47	V	355	VAL
47	V	359	LEU
47	V	377	SER
47	V	378	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (108) such sidechains are listed below:

Mol	Chain	Res	Type
4	z	421	ASN
5	LD	8	GLN
5	LD	47	GLN
5	LD	132	ASN
5	LD	205	ASN
6	LE	109	HIS
6	LE	279	ASN
6	LE	319	ASN
6	LE	345	ASN
7	LF	18	ASN
7	LF	36	HIS
7	LF	45	ASN
7	LF	196	ASN
7	LF	260	GLN
7	LF	304	GLN
8	LG	17	GLN
8	LG	32	GLN

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Mol	Chain	Res	Type
8	LG	57	ASN
8	LG	63	GLN
8	LG	81	HIS
8	LG	244	HIS
9	LH	5	GLN
9	LH	80	ASN
10	LI	52	GLN
10	LI	64	GLN
10	LI	93	ASN
10	LI	200	ASN
11	LJ	28	HIS
11	LJ	85	ASN
12	LK	100	ASN
12	LK	157	ASN
12	LK	162	GLN
13	LL	23	ASN
13	LL	55	ASN
13	LL	59	GLN
13	LL	73	ASN
13	LL	92	HIS
13	LL	133	GLN
14	LM	68	HIS
14	LM	90	GLN
14	LM	101	ASN
14	LM	109	HIS
14	LM	165	GLN
17	LP	11	GLN
17	LP	23	GLN
17	LP	95	GLN
17	LP	138	GLN
17	LP	178	HIS
18	LQ	29	ASN
18	LQ	50	ASN
19	LR	37	ASN
19	LR	55	GLN
19	LR	121	GLN
20	LS	15	HIS
20	LS	23	ASN
21	LT	3	ASN
21	LT	36	ASN
21	LT	144	GLN
22	LU	65	ASN

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Mol	Chain	Res	Type
22	LU	142	GLN
22	LU	157	GLN
23	LV	127	GLN
23	LV	134	GLN
25	LX	24	ASN
26	LY	32	GLN
26	LY	42	GLN
27	LZ	55	ASN
27	LZ	85	GLN
28	La	26	GLN
30	Lc	39	HIS
30	Lc	62	HIS
30	Lc	64	GLN
31	Ld	6	ASN
31	Ld	19	ASN
31	Ld	48	HIS
34	Lg	71	HIS
35	Lh	24	ASN
35	Lh	39	GLN
36	Li	52	GLN
36	Li	61	GLN
36	Li	69	HIS
37	Lj	16	GLN
37	Lj	34	GLN
37	Lj	62	GLN
37	Lj	99	GLN
39	Ll	13	ASN
39	Ll	48	ASN
39	Ll	76	ASN
40	Lm	28	ASN
41	Ln	4	GLN
41	Ln	20	ASN
43	Lq	38	GLN
43	Lq	47	GLN
43	Lq	53	GLN
45	X	145	ASN
45	X	170	GLN
45	X	178	GLN
46	W	117	ASN
46	W	170	GLN
46	W	406	ASN
47	V	47	GLN

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Mol	Chain	Res	Type
47	V	66	GLN
47	V	108	HIS
47	V	176	GLN
47	V	203	GLN
47	V	314	GLN
47	V	358	HIS
47	V	451	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	3009/3396 (88%)	489 (16%)	37 (1%)
2	B	120/121 (99%)	8 (6%)	0
3	C	157/158 (99%)	25 (15%)	1 (0%)
All	All	3286/3675 (89%)	522 (15%)	38 (1%)

All (522) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	13	A
1	A	14	U
1	A	26	A
1	A	40	A
1	A	43	A
1	A	49	A
1	A	59	G
1	A	60	A
1	A	65	A
1	A	66	A
1	A	73	C
1	A	74	G
1	A	77	A
1	A	92	G
1	A	99	A
1	A	110	G
1	A	111	C
1	A	116	A
1	A	117	U
1	A	121	A
1	A	122	A
1	A	135	C

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Mol	Chain	Res	Type
1	A	136	G
1	A	155	G
1	A	156	G
1	A	157	A
1	A	166	C
1	A	187	A
1	A	190	U
1	A	191	U
1	A	200	C
1	A	206	G
1	A	210	U
1	A	211	A
1	A	213	A
1	A	218	G
1	A	219	A
1	A	234	G
1	A	239	G
1	A	240	U
1	A	241	G
1	A	242	C
1	A	243	G
1	A	257	U
1	A	269	G
1	A	270	U
1	A	283	G
1	A	286	U
1	A	295	A
1	A	305	U
1	A	329	U
1	A	330	G
1	A	339	C
1	A	350	C
1	A	351	A
1	A	376	G
1	A	395	A
1	A	399	A
1	A	401	U
1	A	402	A
1	A	403	C
1	A	404	G
1	A	420	G
1	A	421	G

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Mol	Chain	Res	Type
1	A	422	A
1	A	438	A
1	A	503	C
1	A	518	G
1	A	520	U
1	A	521	A
1	A	523	A
1	A	533	A
1	A	535	G
1	A	543	C
1	A	544	C
1	A	545	U
1	A	546	C
1	A	549	U
1	A	555	U
1	A	557	A
1	A	559	A
1	A	560	G
1	A	579	G
1	A	592	A
1	A	604	G
1	A	609	G
1	A	611	A
1	A	620	U
1	A	621	A
1	A	636	C
1	A	637	C
1	A	638	C
1	A	649	A
1	A	662	U
1	A	677	A
1	A	681	U
1	A	683	U
1	A	691	A
1	A	705	A
1	A	712	G
1	A	715	A
1	A	716	A
1	A	719	U
1	A	720	A
1	A	721	G
1	A	727	G

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Mol	Chain	Res	Type
1	A	742	G
1	A	758	C
1	A	764	U
1	A	765	C
1	A	766	U
1	A	767	U
1	A	776	U
1	A	779	G
1	A	781	G
1	A	785	G
1	A	787	G
1	A	806	A
1	A	808	A
1	A	817	A
1	A	830	A
1	A	845	G
1	A	849	C
1	A	861	C
1	A	874	U
1	A	879	U
1	A	896	A
1	A	907	G
1	A	908	G
1	A	914	A
1	A	916	G
1	A	917	A
1	A	921	A
1	A	923	C
1	A	924	G
1	A	937	G
1	A	944	C
1	A	959	C
1	A	960	U
1	A	974	G
1	A	980	A
1	A	981	U
1	A	982	C
1	A	1002	A
1	A	1010	G
1	A	1047	A
1	A	1049	C
1	A	1063	G

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Mol	Chain	Res	Type
1	A	1064	A
1	A	1065	A
1	A	1072	G
1	A	1081	U
1	A	1093	A
1	A	1094	U
1	A	1095	U
1	A	1097	G
1	A	1098	A
1	A	1103	A
1	A	1104	G
1	A	1117	G
1	A	1131	G
1	A	1143	A
1	A	1144	U
1	A	1159	A
1	A	1180	A
1	A	1181	U
1	A	1192	C
1	A	1193	A
1	A	1196	C
1	A	1201	C
1	A	1202	A
1	A	1208	U
1	A	1209	G
1	A	1217	A
1	A	1220	U
1	A	1222	G
1	A	1227	C
1	A	1230	G
1	A	1282	G
1	A	1284	C
1	A	1287	A
1	A	1308	A
1	A	1309	U
1	A	1313	G
1	A	1330	A
1	A	1331	U
1	A	1348	U
1	A	1349	G
1	A	1351	U
1	A	1356	U

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Mol	Chain	Res	Type
1	A	1357	G
1	A	1386	A
1	A	1399	A
1	A	1400	G
1	A	1418	A
1	A	1419	A
1	A	1434	G
1	A	1437	C
1	A	1446	A
1	A	1450	G
1	A	1475	A
1	A	1481	A
1	A	1483	G
1	A	1484	U
1	A	1503	A
1	A	1508	C
1	A	1527	C
1	A	1536	G
1	A	1542	G
1	A	1546	A
1	A	1556	C
1	A	1560	G
1	A	1563	C
1	A	1564	U
1	A	1573	G
1	A	1574	C
1	A	1575	A
1	A	1576	G
1	A	1580	A
1	A	1583	A
1	A	1589	A
1	A	1606	U
1	A	1620	U
1	A	1621	A
1	A	1627	U
1	A	1629	U
1	A	1639	C
1	A	1643	A
1	A	1645	U
1	A	1657	C
1	A	1683	A
1	A	1688	U

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Mol	Chain	Res	Type
1	A	1696	A
1	A	1717	U
1	A	1724	U
1	A	1725	C
1	A	1728	G
1	A	1741	A
1	A	1742	U
1	A	1750	A
1	A	1751	G
1	A	1770	G
1	A	1775	G
1	A	1779	C
1	A	1780	G
1	A	1788	C
1	A	1797	A
1	A	1808	G
1	A	1820	U
1	A	1821	U
1	A	1839	A
1	A	1840	U
1	A	1841	A
1	A	1842	A
1	A	1846	C
1	A	1849	C
1	A	1866	C
1	A	1867	A
1	A	1879	A
1	A	1881	A
1	A	1893	A
1	A	1906	G
1	A	1943	C
1	A	1953	G
1	A	1954	G
1	A	2094	C
1	A	2095	G
1	A	2100	A
1	A	2101	C
1	A	2102	U
1	A	2110	G
1	A	2111	G
1	A	2112	U
1	A	2113	A

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Mol	Chain	Res	Type
1	A	2121	G
1	A	2122	G
1	A	2131	A
1	A	2140	U
1	A	2144	A
1	A	2158	A
1	A	2166	A
1	A	2169	G
1	A	2170	U
1	A	2206	G
1	A	2207	A
1	A	2209	U
1	A	2210	G
1	A	2223	A
1	A	2249	G
1	A	2250	G
1	A	2252	A
1	A	2255	A
1	A	2256	A
1	A	2260	U
1	A	2261	G
1	A	2262	A
1	A	2265	C
1	A	2267	C
1	A	2268	U
1	A	2269	U
1	A	2270	A
1	A	2272	G
1	A	2273	G
1	A	2279	A
1	A	2281	A
1	A	2282	U
1	A	2307	G
1	A	2310	U
1	A	2313	A
1	A	2314	U
1	A	2315	G
1	A	2318	U
1	A	2325	G
1	A	2334	U
1	A	2335	G
1	A	2336	U

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Mol	Chain	Res	Type
1	A	2372	A
1	A	2373	A
1	A	2374	C
1	A	2375	G
1	A	2385	G
1	A	2388	U
1	A	2393	G
1	A	2394	G
1	A	2397	A
1	A	2402	A
1	A	2403	G
1	A	2404	A
1	A	2411	U
1	A	2418	G
1	A	2419	A
1	A	2437	G
1	A	2440	G
1	A	2514	U
1	A	2515	A
1	A	2522	G
1	A	2525	G
1	A	2526	C
1	A	2531	C
1	A	2532	U
1	A	2544	U
1	A	2549	G
1	A	2551	U
1	A	2552	C
1	A	2554	A
1	A	2555	G
1	A	2559	U
1	A	2561	A
1	A	2569	A
1	A	2570	U
1	A	2572	C
1	A	2573	G
1	A	2585	G
1	A	2593	A
1	A	2594	C
1	A	2595	A
1	A	2606	G
1	A	2607	G

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Mol	Chain	Res	Type
1	A	2614	G
1	A	2619	G
1	A	2629	U
1	A	2635	A
1	A	2652	U
1	A	2656	A
1	A	2664	C
1	A	2672	G
1	A	2674	A
1	A	2677	G
1	A	2689	A
1	A	2691	A
1	A	2694	A
1	A	2696	A
1	A	2713	U
1	A	2714	G
1	A	2719	U
1	A	2728	G
1	A	2729	U
1	A	2737	C
1	A	2749	G
1	A	2753	G
1	A	2762	A
1	A	2772	C
1	A	2777	G
1	A	2778	G
1	A	2780	A
1	A	2796	G
1	A	2800	G
1	A	2801	A
1	A	2803	A
1	A	2810	C
1	A	2814	G
1	A	2816	G
1	A	2817	A
1	A	2818	U
1	A	2838	A
1	A	2842	U
1	A	2845	A
1	A	2849	C
1	A	2856	G
1	A	2867	C

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Mol	Chain	Res	Type
1	A	2871	G
1	A	2872	A
1	A	2887	A
1	A	2889	C
1	A	2898	G
1	A	2899	C
1	A	2914	G
1	A	2923	U
1	A	2929	C
1	A	2935	U
1	A	2936	A
1	A	2947	G
1	A	2955	U
1	A	2957	G
1	A	2964	G
1	A	2971	A
1	A	2983	C
1	A	2990	G
1	A	2996	U
1	A	2997	G
1	A	3003	G
1	A	3012	A
1	A	3056	U
1	A	3057	U
1	A	3058	U
1	A	3059	G
1	A	3078	U
1	A	3079	U
1	A	3086	A
1	A	3092	C
1	A	3093	C
1	A	3101	G
1	A	3104	U
1	A	3116	G
1	A	3117	C
1	A	3119	U
1	A	3122	A
1	A	3129	A
1	A	3130	A
1	A	3131	U
1	A	3142	A
1	A	3143	C

Continued on next page...

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Mol	Chain	Res	Type
1	A	3165	A
1	A	3170	A
1	A	3173	G
1	A	3174	A
1	A	3175	U
1	A	3176	G
1	A	3179	U
1	A	3180	A
1	A	3181	C
1	A	3187	A
1	A	3196	U
1	A	3197	G
1	A	3198	U
1	A	3207	U
1	A	3210	A
1	A	3217	C
1	A	3218	A
1	A	3219	G
1	A	3239	G
1	A	3243	A
1	A	3245	A
1	A	3247	G
1	A	3249	C
1	A	3259	U
1	A	3270	U
1	A	3273	A
1	A	3276	G
1	A	3281	U
1	A	3287	U
1	A	3288	G
1	A	3289	G
1	A	3294	A
1	A	3295	A
1	A	3304	U
1	A	3316	A
1	A	3319	U
1	A	3320	A
1	A	3331	U
1	A	3334	U
1	A	3345	G
1	A	3363	U
1	A	3369	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	3378	C
1	A	3382	U
1	A	3386	G
1	A	3389	U
1	A	3390	G
2	B	7	G
2	B	10	C
2	B	22	A
2	B	35	C
2	B	39	C
2	B	65	G
2	B	102	A
2	B	112	G
3	C	34	U
3	C	35	C
3	C	48	A
3	C	59	A
3	C	62	C
3	C	63	G
3	C	80	A
3	C	81	U
3	C	82	U
3	C	83	C
3	C	84	C
3	C	85	G
3	C	86	U
3	C	87	G
3	C	90	U
3	C	91	C
3	C	95	G
3	C	104	A
3	C	106	C
3	C	112	U
3	C	125	U
3	C	126	A
3	C	138	A
3	C	148	G
3	C	152	G

All (38) RNA pucker outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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Mol	Chain	Res	Type
1	A	13	A
1	A	73	C
1	A	186	U
1	A	282	G
1	A	637	C
1	A	763	G
1	A	916	G
1	A	1064	A
1	A	1097	G
1	A	1208	U
1	A	1307	G
1	A	1348	U
1	A	1355	A
1	A	1483	G
1	A	1562	C
1	A	1820	U
1	A	1821	U
1	A	2110	G
1	A	2112	U
1	A	2249	G
1	A	2264	U
1	A	2266	U
1	A	2513	U
1	A	2525	G
1	A	2549	G
1	A	2898	G
1	A	2996	U
1	A	3056	U
1	A	3057	U
1	A	3078	U
1	A	3121	U
1	A	3196	U
1	A	3218	A
1	A	3269	U
1	A	3272	C
1	A	3280	U
1	A	3319	U
3	C	85	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](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
48	3HE	A	3401	-	21,21,21	0.47	0	23,30,30	0.90	1 (4%)

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
48	3HE	A	3401	-	-	2/8/36/36	0/2/2/2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	A	3401	3HE	O3-C7-C8	2.19	113.54	109.15

There are no chirality outliers.

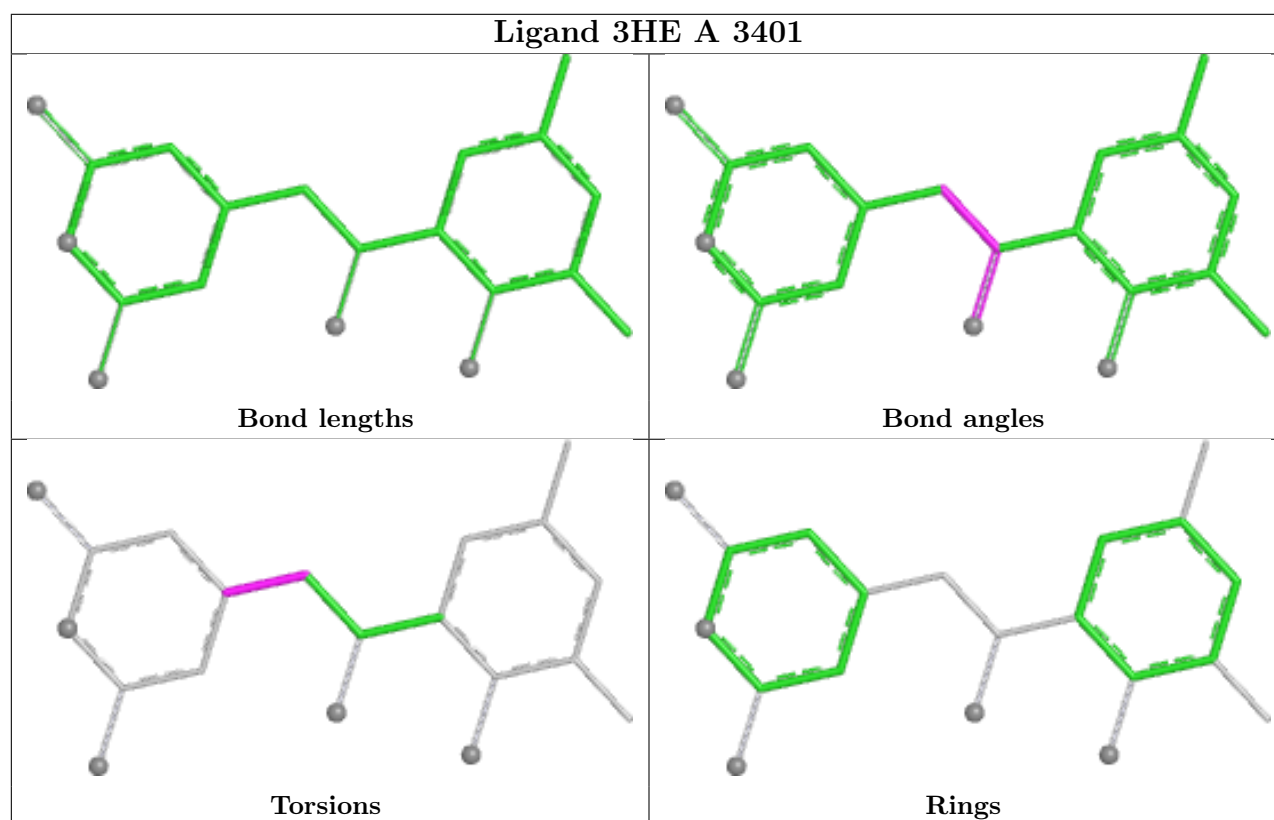
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
48	A	3401	3HE	C7-C8-C9-C10
48	A	3401	3HE	C7-C8-C9-C13

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 ⓘ

There are no chain breaks in this entry.

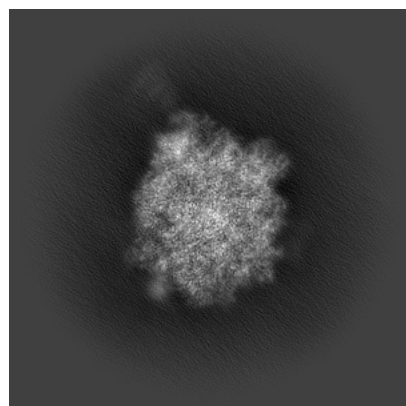
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72799. These allow visual inspection of the internal detail of the map and identification of artifacts.

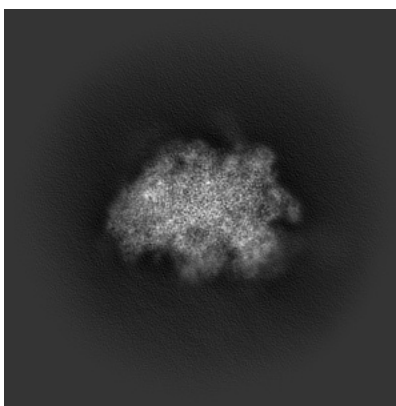
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

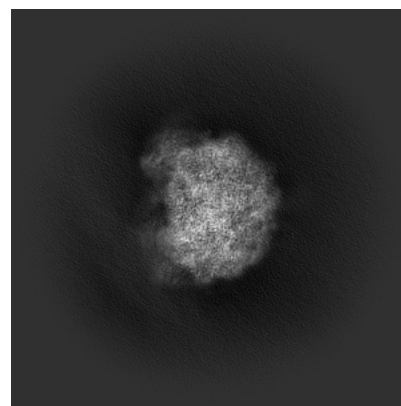
6.1.1 Primary map



X

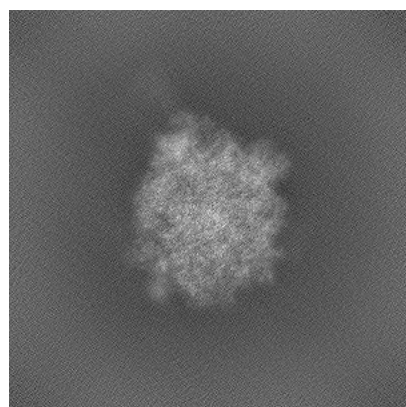


Y

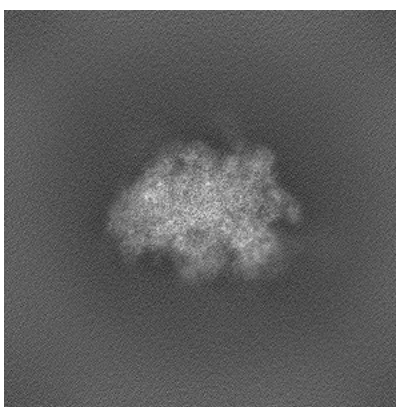


Z

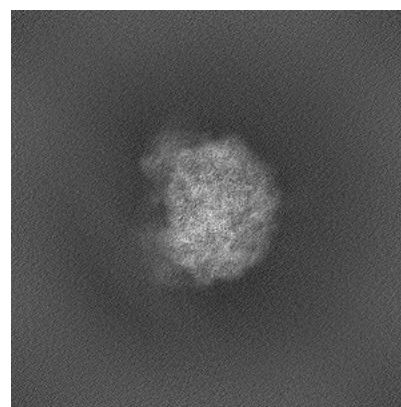
6.1.2 Raw map



X



Y

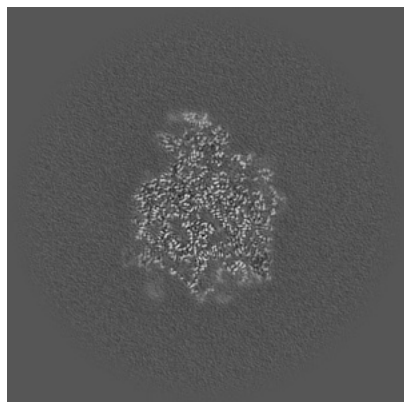


Z

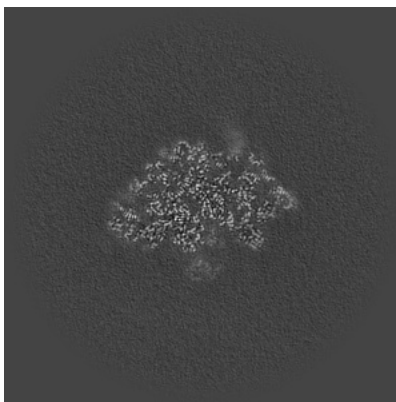
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

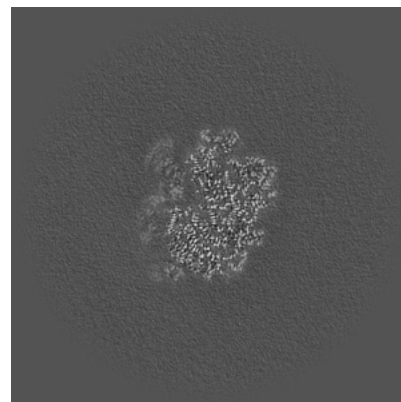
6.2.1 Primary map



X Index: 300

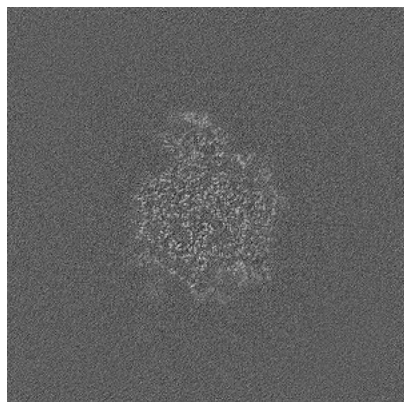


Y Index: 300

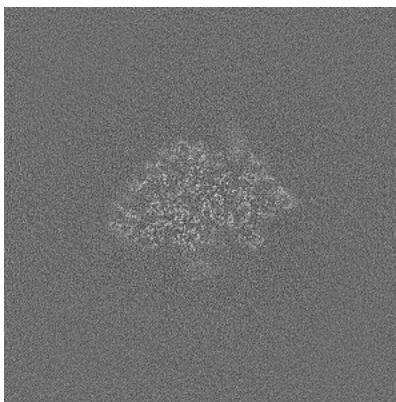


Z Index: 300

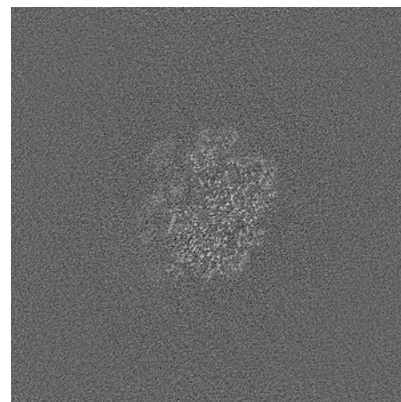
6.2.2 Raw map



X Index: 300



Y Index: 300

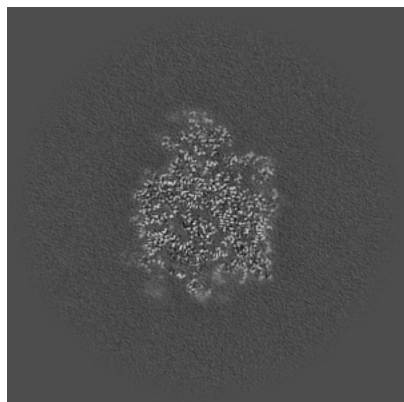


Z Index: 300

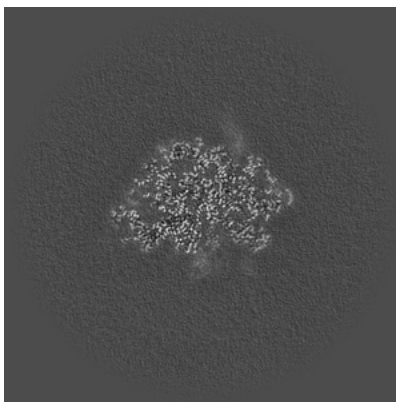
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

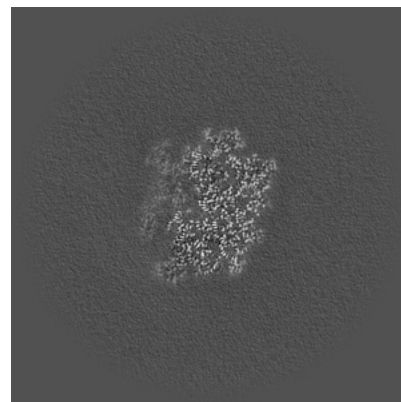
6.3.1 Primary map



X Index: 303

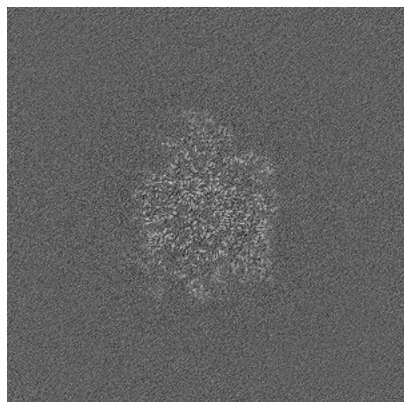


Y Index: 308

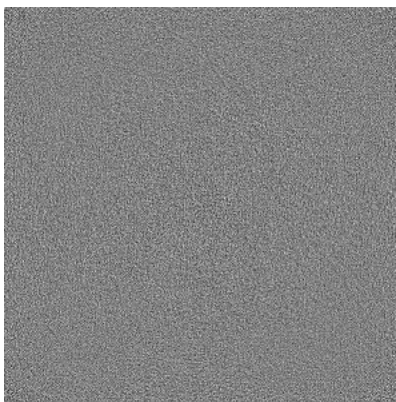


Z Index: 305

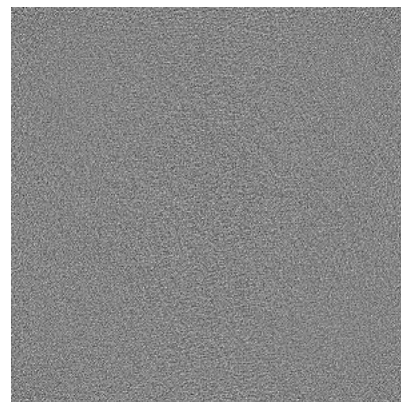
6.3.2 Raw map



X Index: 304



Y Index: 0

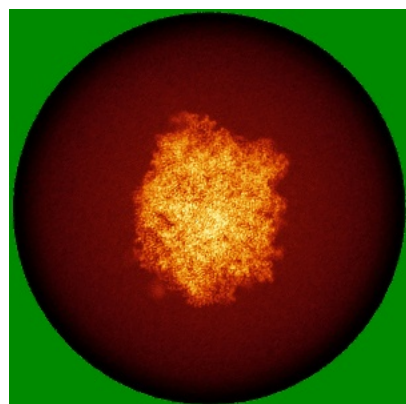


Z Index: 0

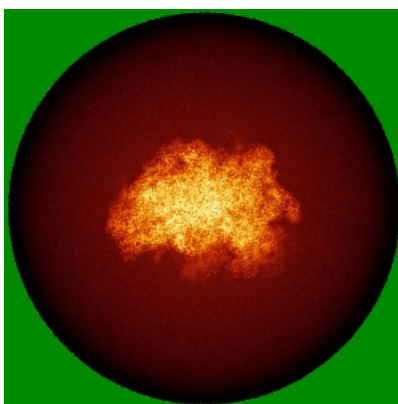
The images above show the largest variance slices of the map in three orthogonal directions.

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

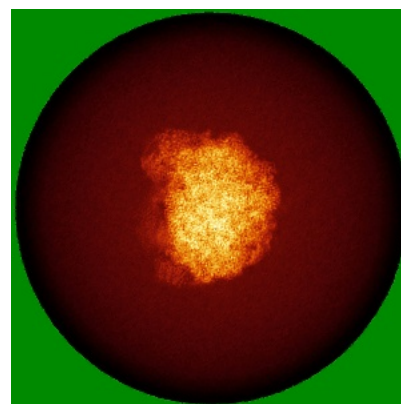
6.4.1 Primary map



X

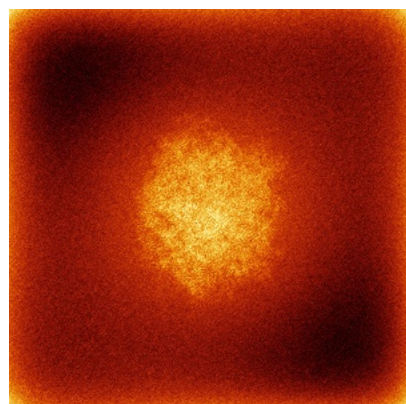


Y

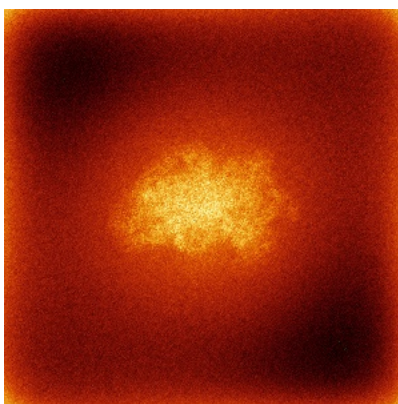


Z

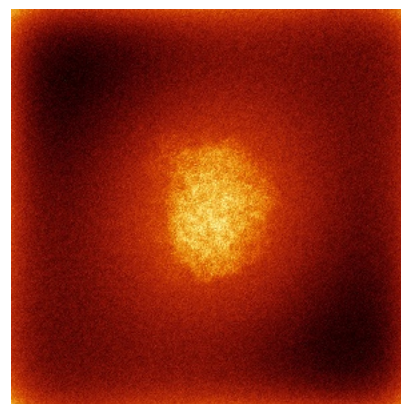
6.4.2 Raw map



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



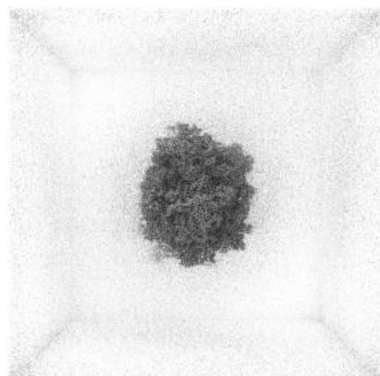
Y



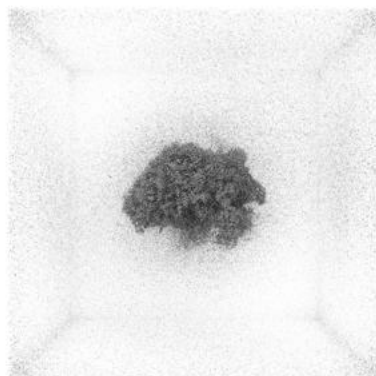
Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

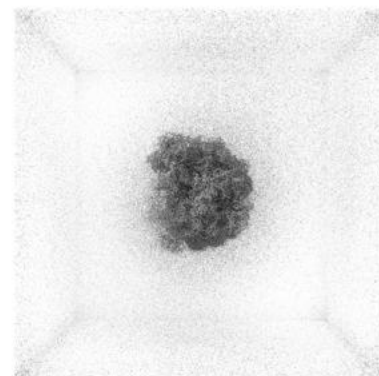
6.5.2 Raw map



X



Y



Z

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

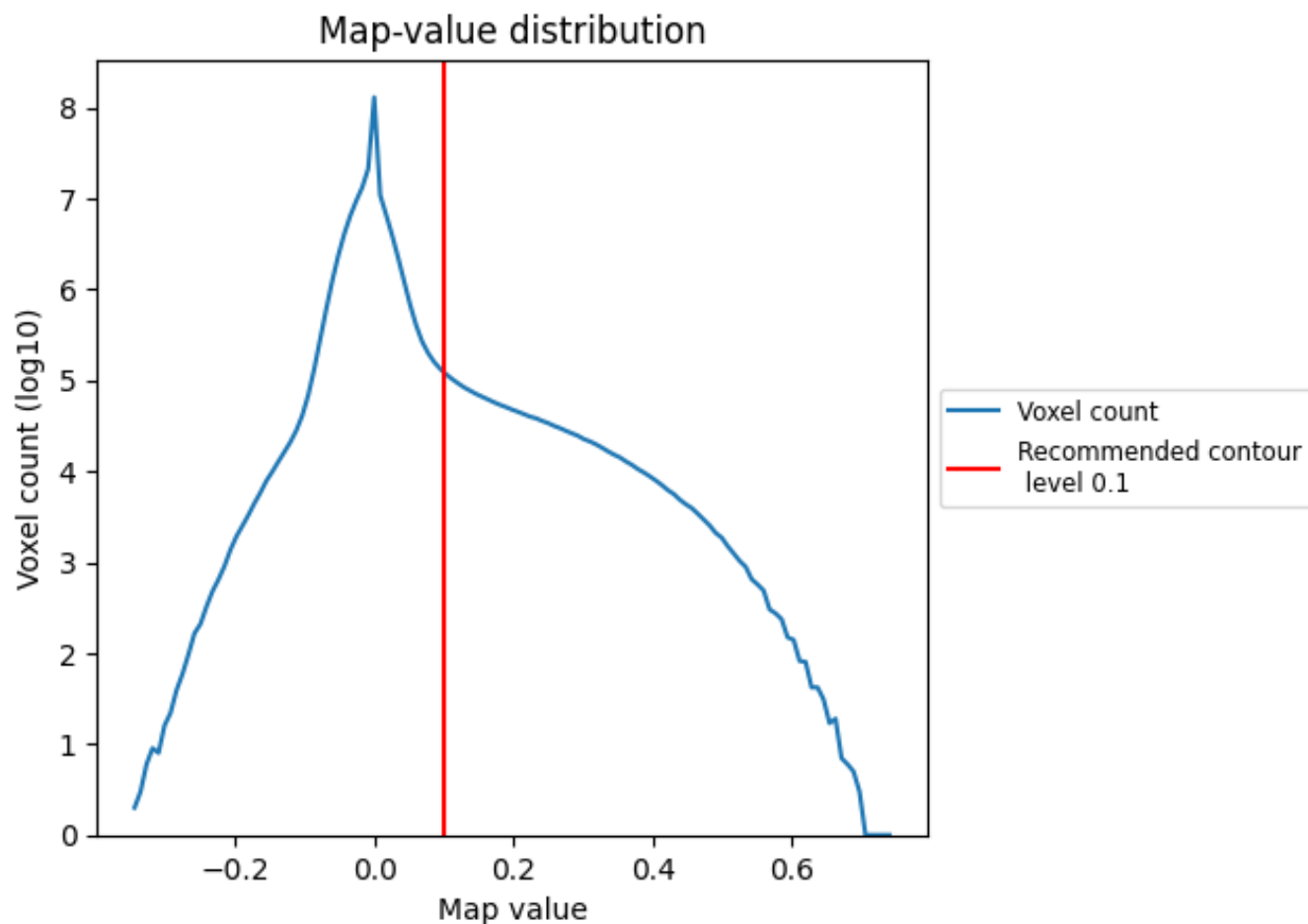
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

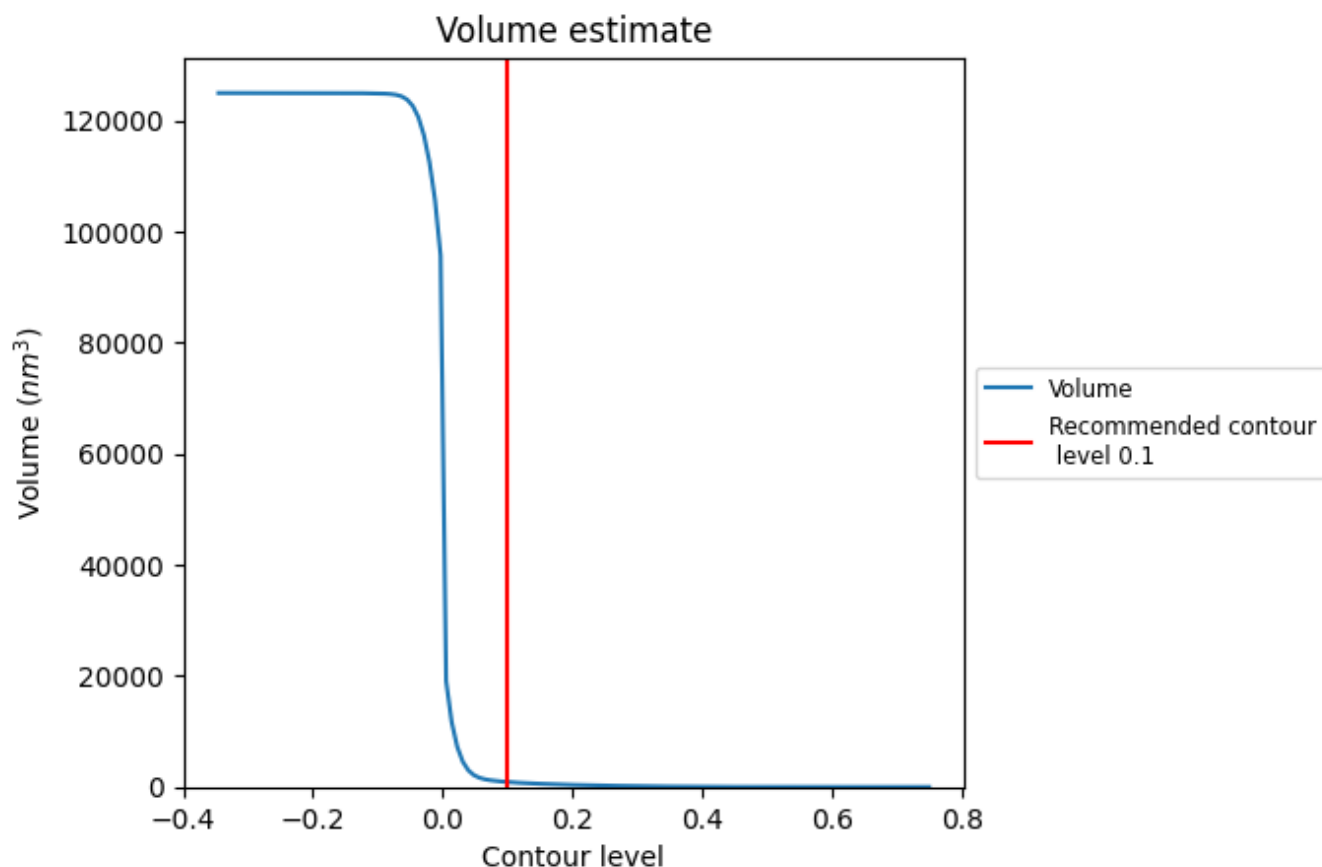
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

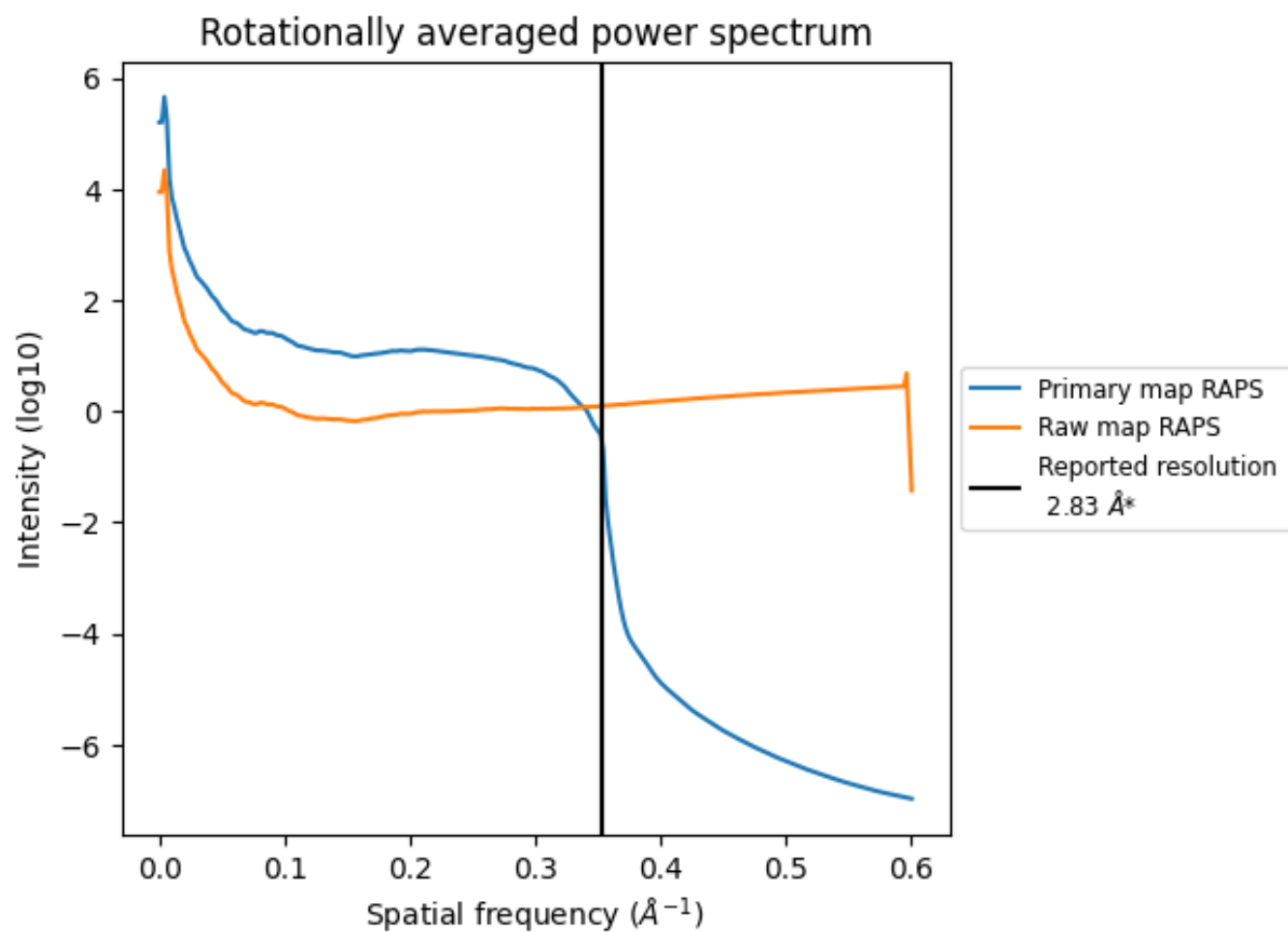
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 891 nm³; this corresponds to an approximate mass of 805 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 ⓘ

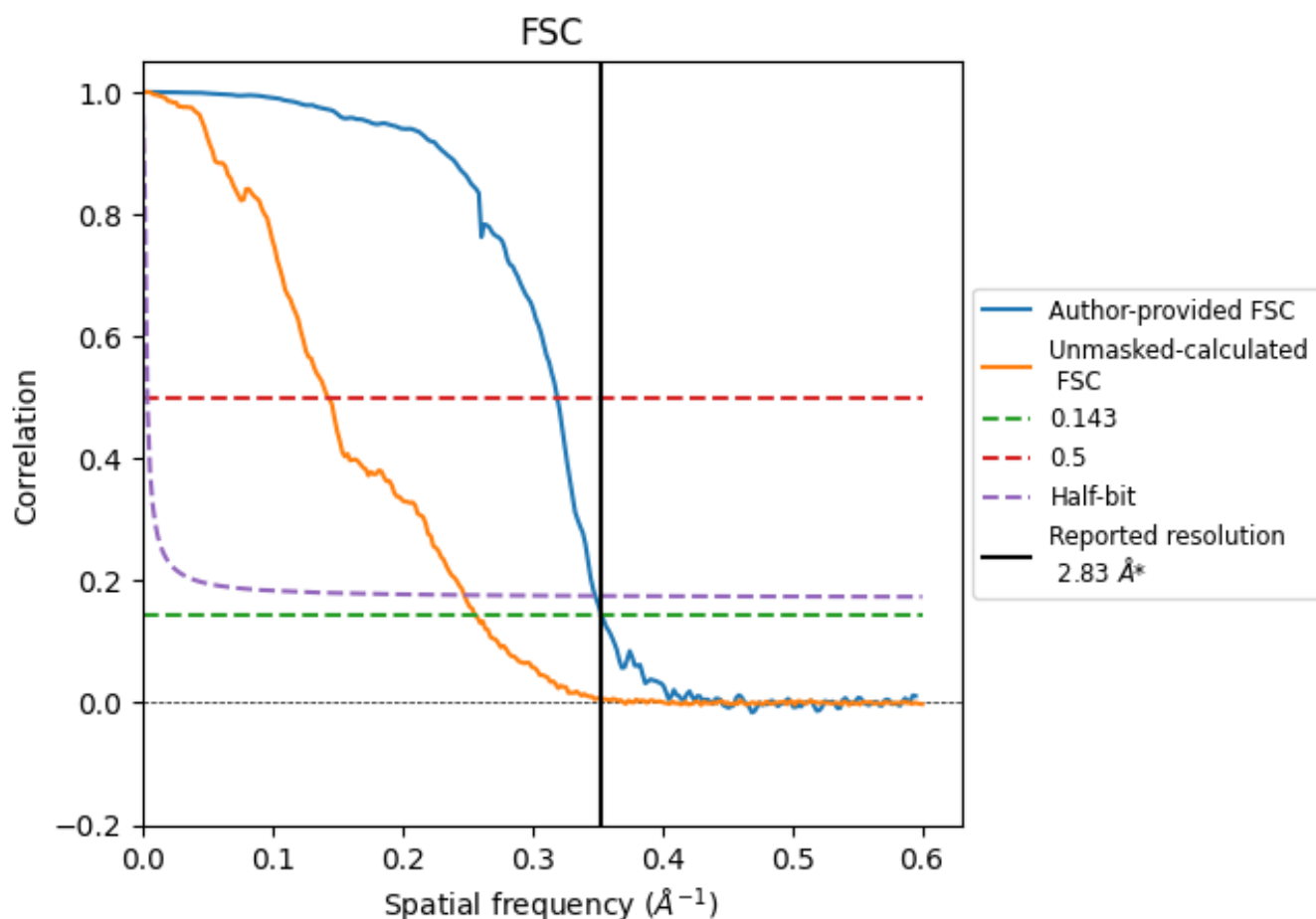


*Reported resolution corresponds to spatial frequency of 0.353 $\text{\AA}^{-1}$

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 0.353 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

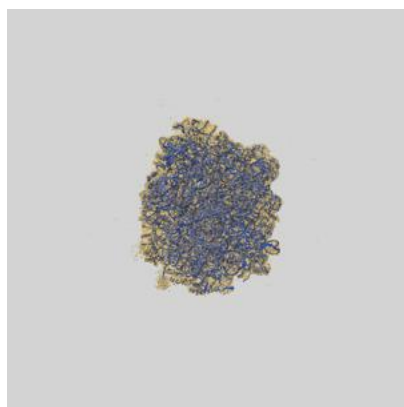
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.83	-	-
Author-provided FSC curve	2.83	3.13	2.87
Unmasked-calculated*	3.91	6.98	4.04

*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 3.91 differs from the reported value 2.83 by more than 10 %

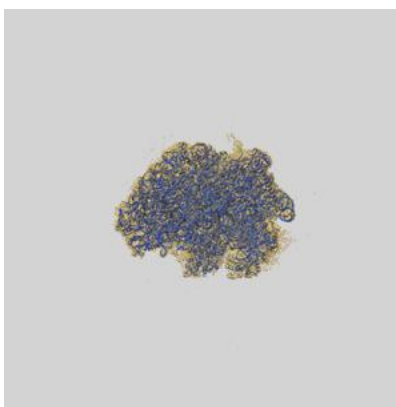
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-72799 and PDB model 9YDB. Per-residue inclusion information can be found in section [3](#) on page [13](#).

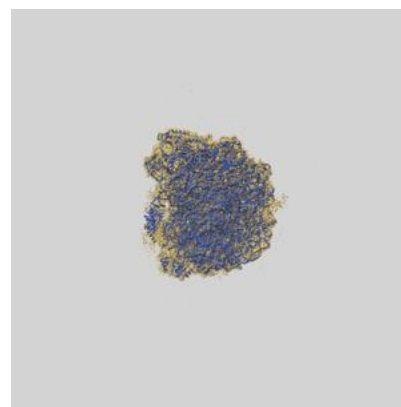
9.1 Map-model overlay [i](#)



X



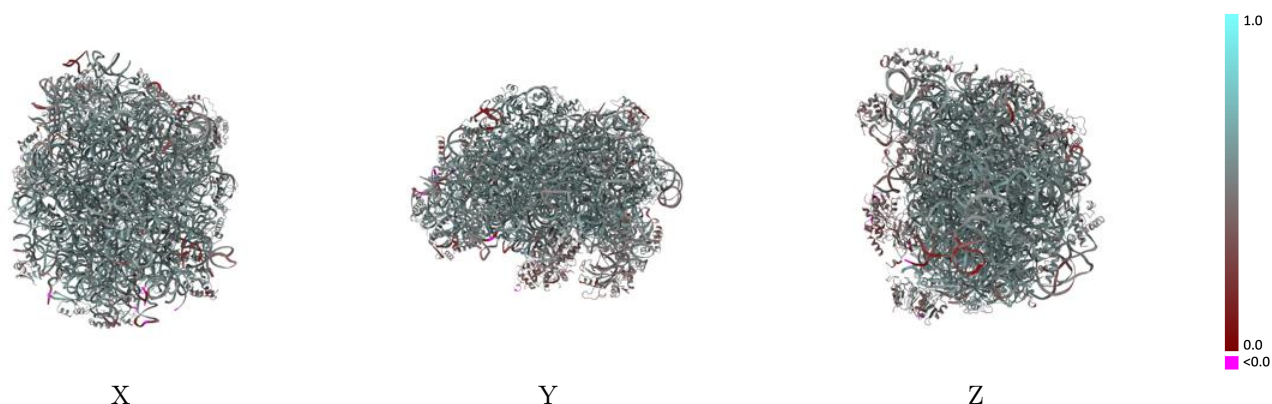
Y



Z

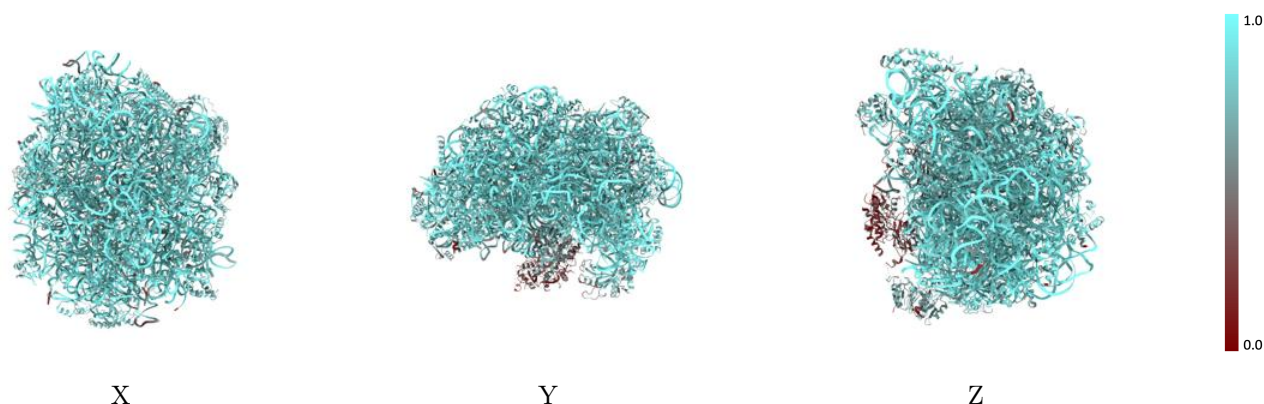
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



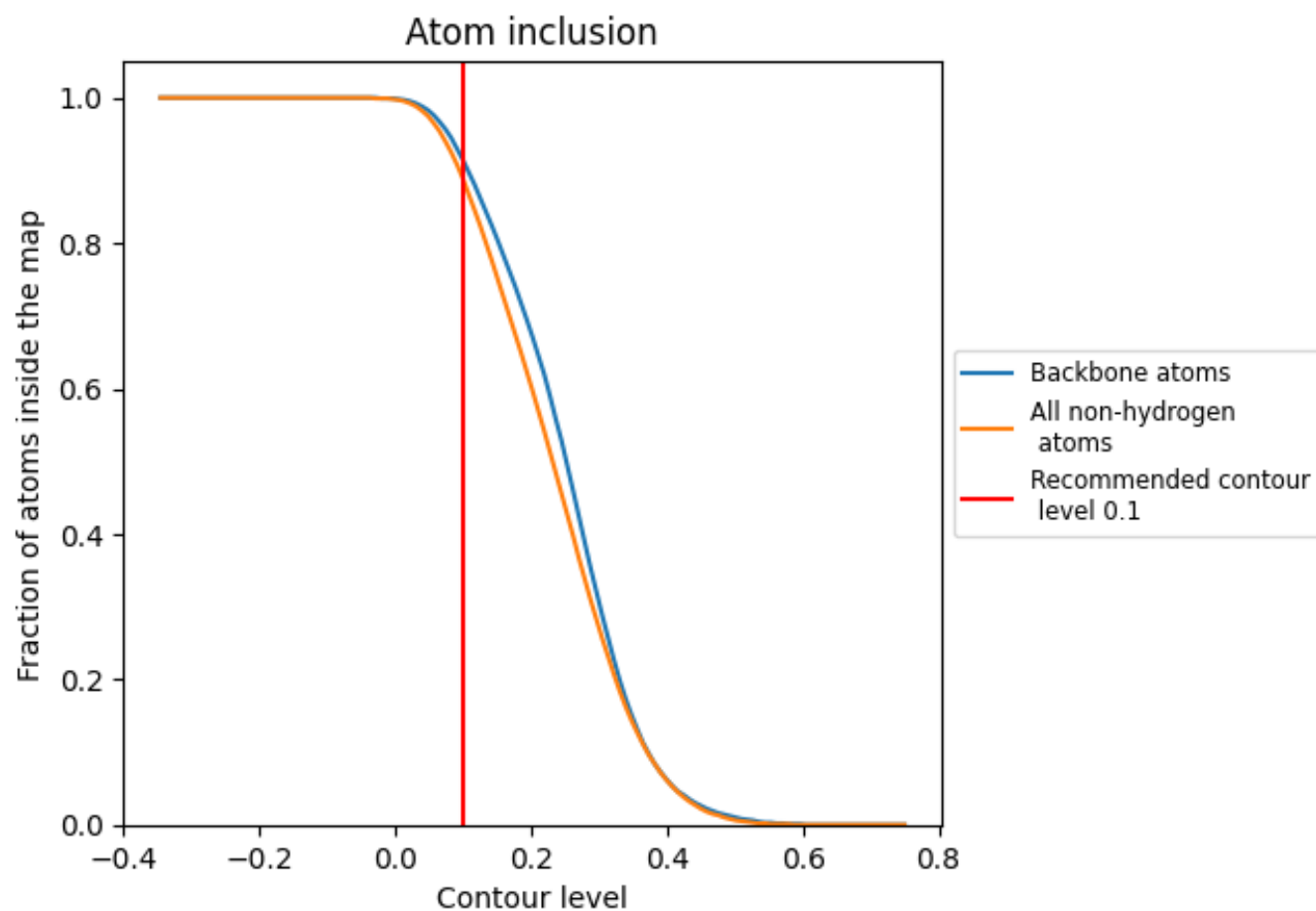
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 89% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8880	 0.5350
A	 0.9460	 0.5460
B	 0.9600	 0.5240
C	 0.9590	 0.5570
LD	 0.8990	 0.5650
LE	 0.9000	 0.5600
LF	 0.8860	 0.5450
LG	 0.8220	 0.4860
LH	 0.8170	 0.5050
LI	 0.8620	 0.5390
LJ	 0.8370	 0.5120
LK	 0.8610	 0.5250
LL	 0.8260	 0.5340
LM	 0.6940	 0.4240
LN	 0.8550	 0.5330
LO	 0.8560	 0.5380
LP	 0.9260	 0.5770
LQ	 0.9060	 0.5580
LR	 0.9160	 0.5700
LS	 0.8720	 0.5540
LT	 0.8850	 0.5550
LU	 0.8750	 0.5510
LV	 0.8570	 0.5540
LW	 0.8310	 0.4970
LX	 0.8540	 0.5460
LY	 0.8610	 0.5500
LZ	 0.8880	 0.5520
La	 0.8800	 0.5420
Lb	 0.8370	 0.5240
Lc	 0.8940	 0.5530
Ld	 0.8520	 0.5240
Le	 0.8210	 0.5100
Lf	 0.8750	 0.5520
Lg	 0.8720	 0.5610
Lh	 0.9000	 0.5730



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Chain	Atom inclusion	Q-score
Li	 0.8850	 0.5600
Lj	 0.8830	 0.5390
Lk	 0.8210	 0.5180
Ll	 0.9370	 0.5860
Lm	 0.8330	 0.5350
Ln	 0.9040	 0.5780
Lo	 0.8790	 0.5390
Lq	 0.8720	 0.5520
Lr	 0.8630	 0.5460
V	 0.4520	 0.4160
W	 0.3460	 0.3800
X	 0.6420	 0.4520
z	 0.7010	 0.4960