



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 01:00 AM UTC

PDB ID : 8XXL / pdb_00008xxl
EMDB ID : EMD-38752
Title : Cryo-EM structure of the human 40S ribosome with PDCD4
Authors : Ye, X.; Huang, Z.; Li, Y.; Wang, M.; Cheng, J.
Deposited on : 2024-01-18
Resolution : 2.90 Å(reported)
Based on initial model : 6ZVJ

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

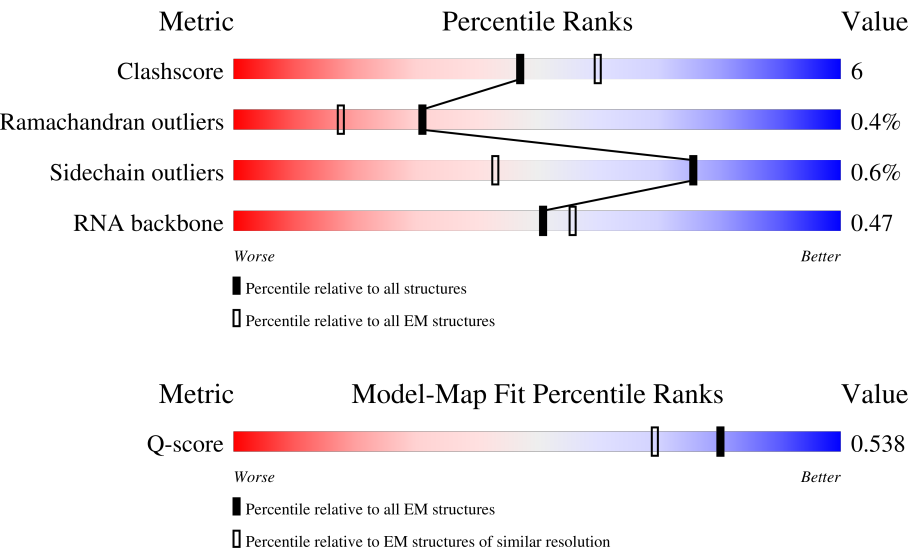
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.90 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	13054 (2.40 - 3.40)

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	Ln	25	
2	S2	1869	
3	SA	295	

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Mol	Chain	Length	Quality of chain
4	SB	264	
5	SD	243	
6	SE	263	
7	SF	204	
8	SH	194	
9	SI	208	
10	SK	165	
11	SL	158	
12	SP	145	
13	SQ	146	
14	SR	135	
15	SS	152	
16	ST	145	
17	SU	119	
18	SV	83	
19	SX	143	
20	Sa	115	
21	Sc	69	
22	Sd	56	
23	Sg	317	
24	SC	293	
25	SG	249	
26	SJ	194	
27	SM	132	
28	SN	151	

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Mol	Chain	Length	Quality of chain
29	SO	151	
30	SW	130	
31	SY	133	
32	SZ	125	
33	Sb	84	
34	Se	59	
35	Sf	156	
36	CD	469	

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 76240 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Ln	24	Total	C	N	O	S	0	0
			230	139	62	26	3		

- Molecule 2 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	S2	1723	Total	C	N	O	P	0	0
			36538	16298	6533	11984	1723		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	SA	221	Total	C	N	O	S	0	0
			1741	1106	305	322	8		

- Molecule 4 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	SB	214	Total	C	N	O	S	0	0
			1738	1103	310	311	14		

- Molecule 5 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	SD	227	Total	C	N	O	S	0	0
			1765	1125	317	315	8		

- Molecule 6 is a protein called 40S ribosomal protein S4, X isoform.

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

- Molecule 7 is a protein called 40S ribosomal protein S5.

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

- Molecule 8 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	SH	186	Total	C	N	O	S	0	0
			1497	956	274	266	1		

- Molecule 9 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	SI	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

- Molecule 10 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	SK	98	Total	C	N	O	S	0	0
			827	539	148	134	6		

- Molecule 11 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	SL	153	Total	C	N	O	S	0	0
			1247	793	234	214	6		

- Molecule 12 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	SP	121	Total	C	N	O	S	0	0
			985	623	185	170	7		

- Molecule 13 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	SQ	144	Total	C	N	O	S	0	0
			1142	726	216	197	3		

- Molecule 14 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	SR	135	Total	C	N	O	S	0	0
			1090	685	202	198	5		

- Molecule 15 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	SS	145	Total	C	N	O	S	0	0
			1198	751	242	203	2		

- Molecule 16 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	ST	143	Total	C	N	O	S	0	0
			1112	697	214	198	3		

- Molecule 17 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	SU	104	Total	C	N	O	S	0	0
			821	514	155	148	4		

- Molecule 18 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	SV	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 19 is a protein called 40S ribosomal protein S23.

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

- Molecule 20 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Sa	102	Total	C	N	O	S	0	0
			821	512	171	133	5		

- Molecule 21 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Sc	64	Total	C	N	O	S	0	0
			506	308	102	94	2		

- Molecule 22 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Sd	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 23 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Sg	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 24 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	SC	222	Total	C	N	O	S	0	0
			1725	1115	298	302	10		

- Molecule 25 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	SG	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 26 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	SJ	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 27 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	SM	122	Total	C	N	O	S	0	0
			940	590	164	177	9		

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

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

- Molecule 29 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	SO	140	Total	C	N	O	S	0	0
			1049	642	204	197	6		

- Molecule 30 is a protein called 40S ribosomal protein S15a.

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

- Molecule 31 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	SY	131	Total	C	N	O	S	0	0
			1065	673	209	178	5		

- Molecule 32 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	SZ	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 33 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Sb	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 34 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Se	58	Total	C	N	O	S	0	0
			459	284	100	74	1		

- Molecule 35 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Sf	67	Total	C	N	O	S	0	0
			548	346	102	93	7		

- Molecule 36 is a protein called Programmed cell death protein 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	CD	46	Total	C	N	O	0	0
			346	211	66	69		

- Molecule 37 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
37	S2	21	Total	Mg	0
			21	21	
37	SG	1	Total	Mg	0
			1	1	

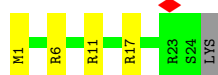
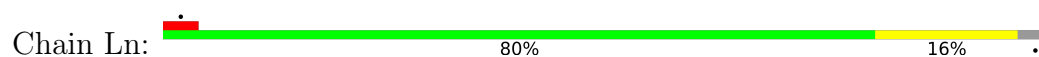
- Molecule 38 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
38	Sa	1	Total	Zn	0
			1	1	
38	Sd	1	Total	Zn	0
			1	1	
38	Sf	1	Total	Zn	0
			1	1	

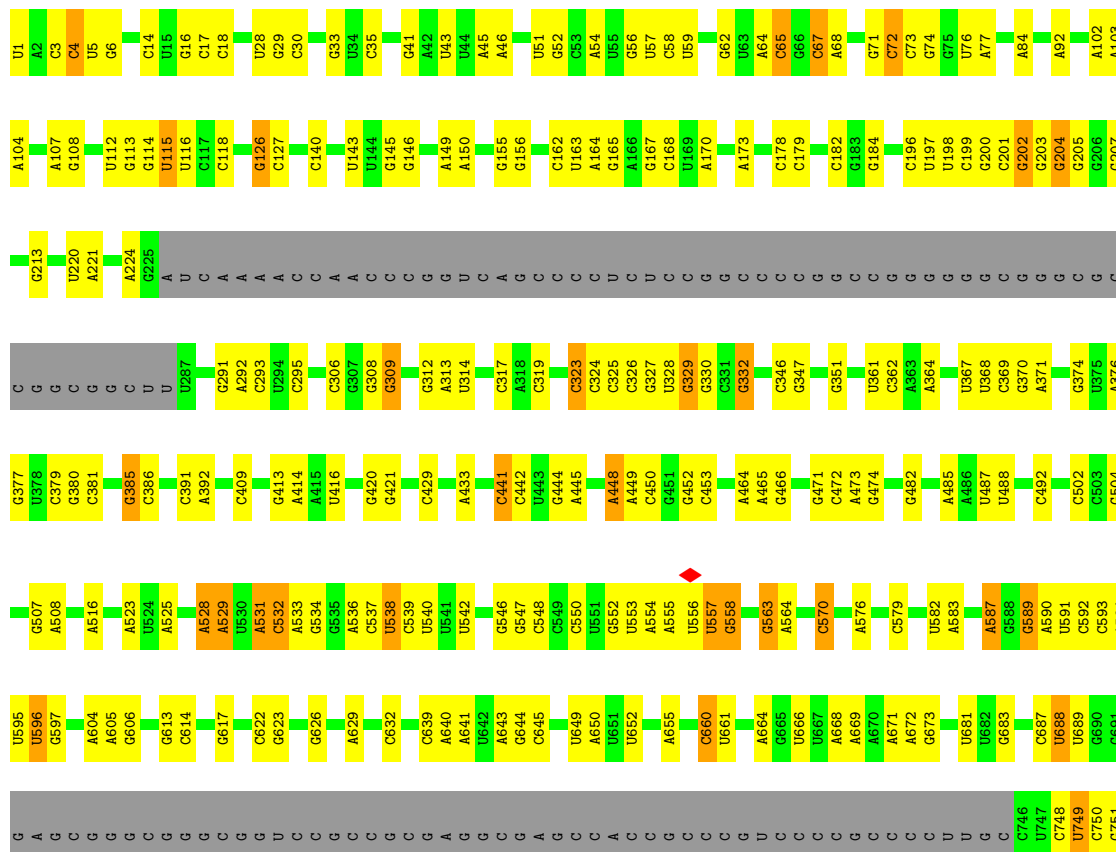
3 Residue-property plots

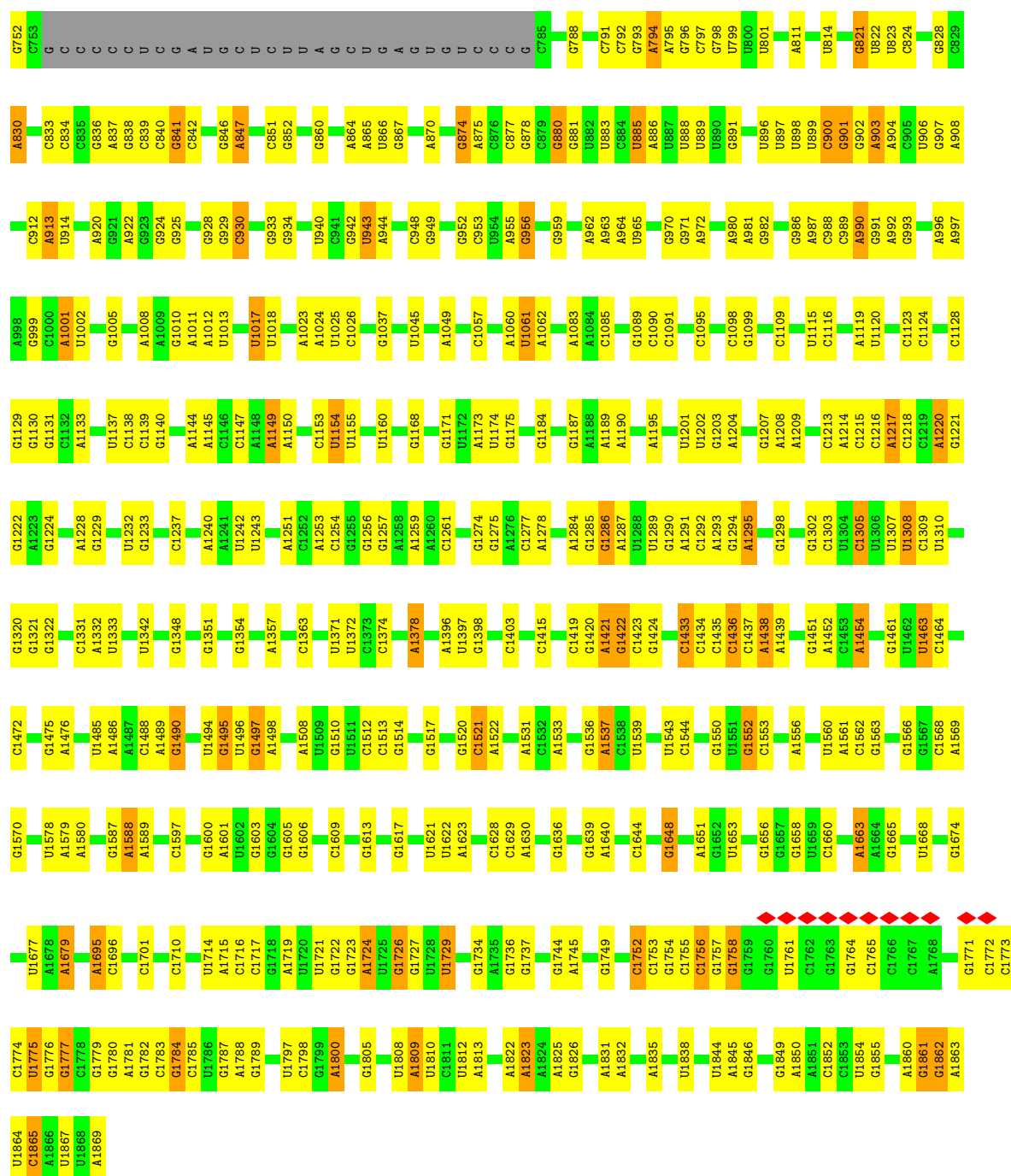
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: 60S ribosomal protein L41



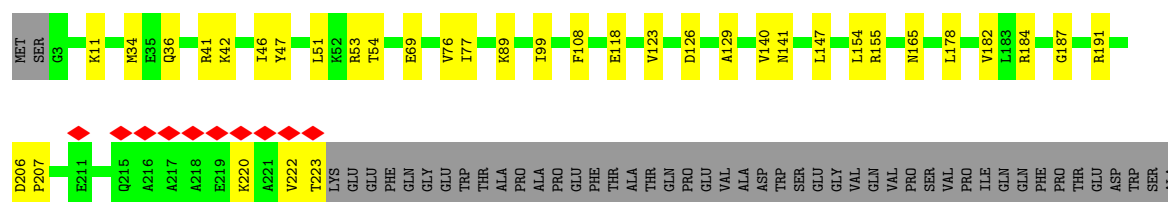
• Molecule 2: 18S rRNA





• Molecule 3: 40S ribosomal protein SA

Chain SA: 63% 12% 25%



GLN
PRO
ALA
THR
GLU
ASP
TRP
SER
ALA
PRO
ALA
THR
THR
GLN
ALA
THR
GLU
TRP
VAL
GLY
ALA
THR
THR
ASP
TRP
SER

• Molecule 4: 40S ribosomal protein S3a

Chain SB:  67% 14% 19%

MET
ALA
GLY
LYS
ASN
LYS
ARG
LEU
THR
LYS
GLY
LYS
LYS
GLY
ALA
LYS
LYS
LYS
V21
V33
A37
N40
I41
R42
M43
I44
R65
D73
L74
Q75
K83
T88
C96
T106
K116
M120
V125
T129
T130
D131
L134
L137
F138

R146
Q149
I150
R151
R162
M172
T173
Q177
T178
N179
K187
R213
K214
V215
L218
K219
P221
K222
E234
GLY
SER
SER
SER
GLY
LYS
ALA
THR
GLY
ASP
GLU
THR
GLY
ALA
LYS
VAL
GLU
ARG
ALA
ASP
GLY
TYR
GLU
PRO
PRO
VAL
GLN
GLU
SER
VAL

• Molecule 5: 40S ribosomal protein S3

Chain SD:  78% 16% 7%

M1
K7
K8
R9
R45
I50
Q56
N57
R64
Q74
F79
E85
L86
R94
R106
L109
L110
L123
V136
V137
G140
K141
K151
F152
I158
V164
V172
R173
H174
V175
L176
L177
R178
Q179
L182
G183
I184
K185
V186
T220

T221
Q226
K227
GLY
LYS
PRO
GLU
PRO
PRO
ALA
MET
PRO
GLN
VAL
PRO
THR
ALA

• Molecule 6: 40S ribosomal protein S4, X isoform

Chain SE:  82% 18%

MET
A2
R11
K16
H17
W18
A28
P31
L38
C41
L44
I45
R51
Y54
V61
M66
I72
T78
D79
Y82
G85
D88
E97
R100
D104
T105
K106
G107
R108
F109
R113
I114
T115
E118
K122
L123
C124

P137
T141
P150
F175
G185
L189
N197
R198
E199
V208
K211
G215
I225
T247
E250
G263

• Molecule 7: 40S ribosomal protein S5

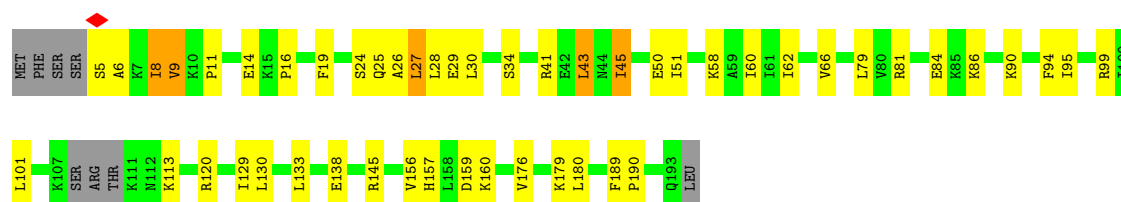
Chain SF:  78% 14% 7%

MET
THR
GLU
TRP
GLU
THR
ALA
ALA
ALA
VAL
ALA
GLU
THR
PRO
D16
T25
D26
D27
V28
K42
E43
Y48
A58
I68
V69
E70
R71
M78
N83
K86
L87
Q110
N114
N118
T126
R127
G132
T133
V134
R135
R136
D140
V141
S142

N148
R164
A181
K193
E197
R204

• Molecule 8: 40S ribosomal protein S7

Chain SH:  70% 23% . .



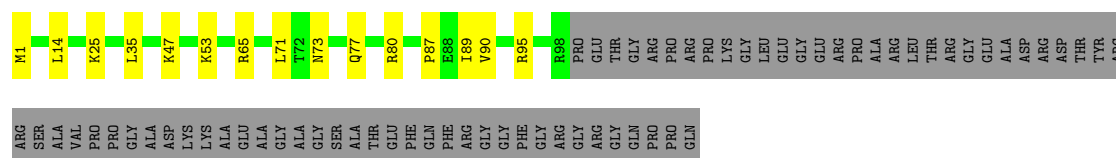
- Molecule 9: 40S ribosomal protein S8

Chain SI: 87% 12%



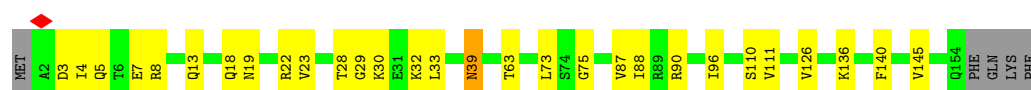
- Molecule 10: 40S ribosomal protein S10

Chain SK: 50% 9% 41%



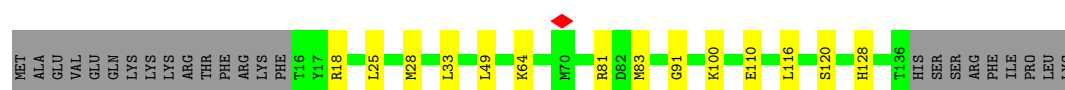
- Molecule 11: 40S ribosomal protein S11

Chain SL: 78% 18%



- Molecule 12: 40S ribosomal protein S15

Chain SP: 74% 10% 17%



- Molecule 13: 40S ribosomal protein S16

Chain SQ: 78% 18%



- Molecule 14: 40S ribosomal protein S17

Chain SR: 93% 7%



- Molecule 15: 40S ribosomal protein S18

Chain SS: 70% 25% 5%



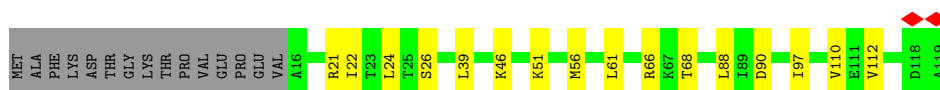
- Molecule 16: 40S ribosomal protein S19

Chain ST: 78% 21% .



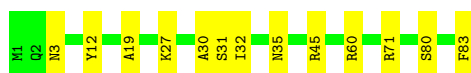
- Molecule 17: 40S ribosomal protein S20

Chain SU: 74% 13% 13%



- Molecule 18: 40S ribosomal protein S21

Chain SV: 84% 16%



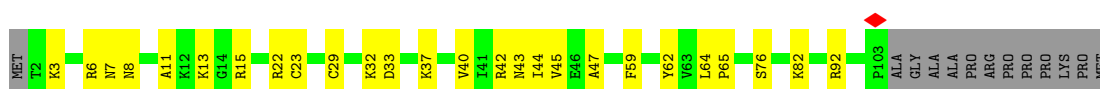
- Molecule 19: 40S ribosomal protein S23

Chain SX: 83% 15% ..

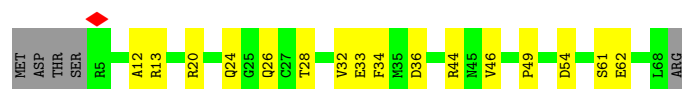


- Molecule 20: 40S ribosomal protein S26

Chain Sa: 66% 23% 11%

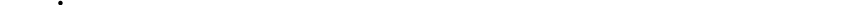


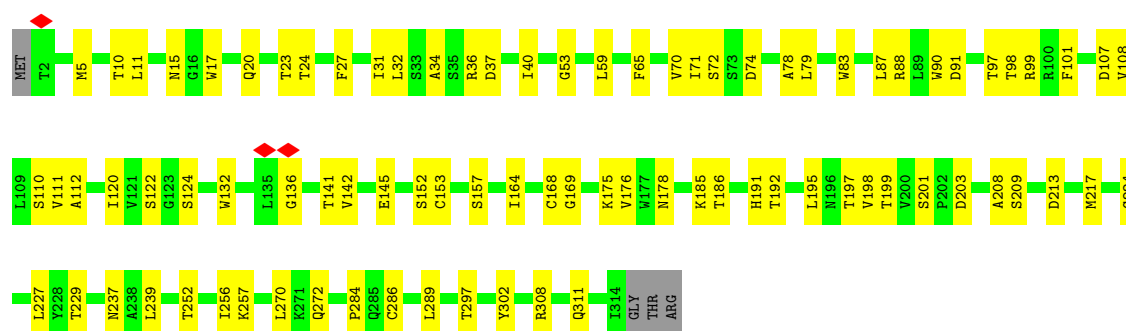
- Molecule 21: 40S ribosomal protein S28

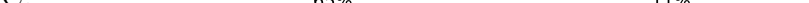


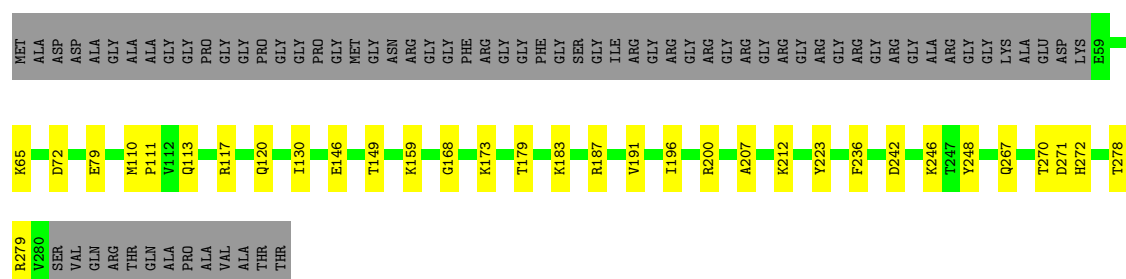
- Chain Sd: 



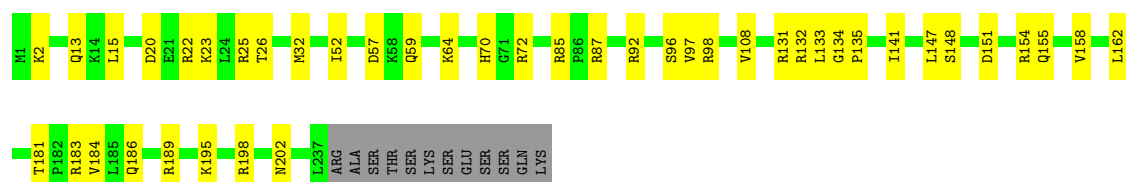
- Chain Sg:  72% 27%



- Chain SC:  65% 11% 24%



- Chain SG: 



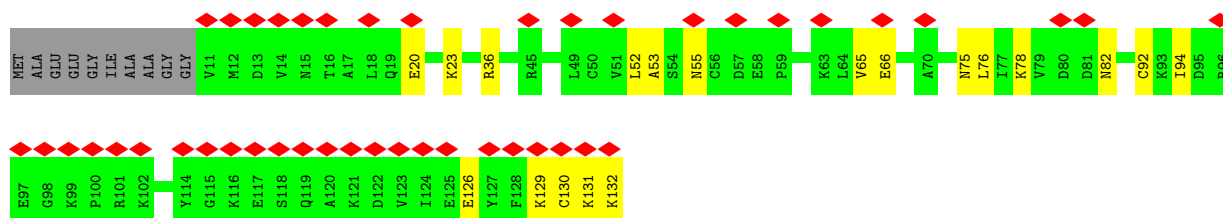
- Molecule 26: 40S ribosomal protein S9

Chain SJ:  86% 9% 5%



- Molecule 27: 40S ribosomal protein S12

Chain SM:  33% 78% 14% 8%



- Molecule 28: 40S ribosomal protein S13

Chain SN:  88% 11%



- Molecule 29: 40S ribosomal protein S14

Chain SO:  75% 17% 7%



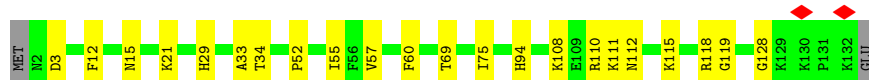
- Molecule 30: 40S ribosomal protein S15a

Chain SW:  89% 10%

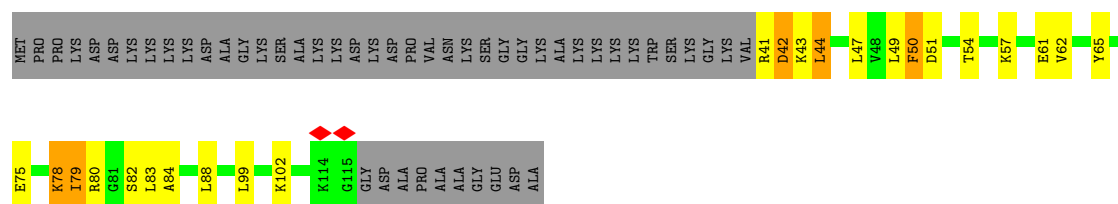


- Molecule 31: 40S ribosomal protein S24

Chain SY:  82% 17%

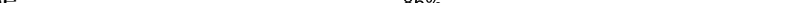


- Molecule 32: 40S ribosomal protein S25

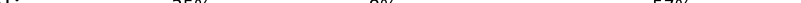


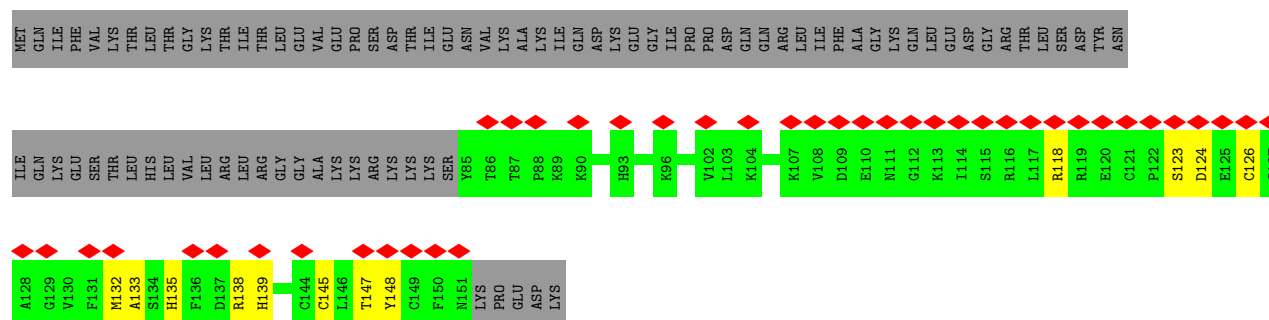
- Chain Sb: 77% 21%

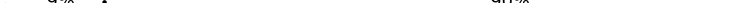


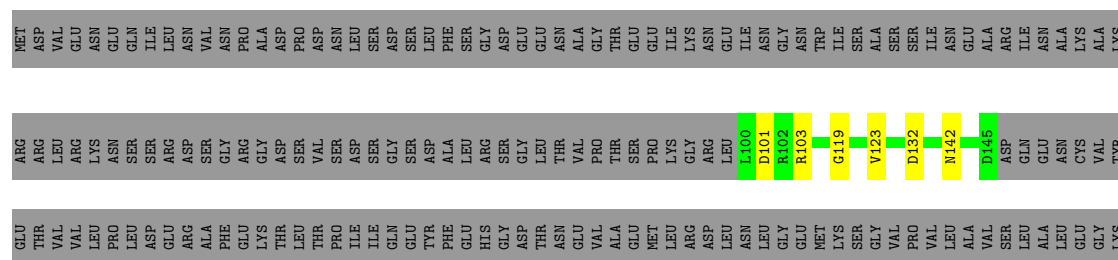
- Chain Se:  86% 12%



- Chain Sf: 



- Chain CD:  9% . 90%



Lys	Ser	Met	Ala
Arg	Ser	Leu	Ser
Phe	Thr	Leu	His
Val	Ile	Lys	Cys
Ser	Thr	Leu	Asn
Leu	Val	Tyr	Thr
Leu	Val	Tyr	Met
Gly	Asp	Leu	Thr
Asp	Gln	Leu	Ser
Gly	Met	Ser	Lys
Gly	Lys	Ser	Lys
Arg	Arg	Asp	Leu
Leu	Gly	Ile	Ser
Leu	Gly	Tyr	Asp
Lys	Tyr	Ser	Asp
Pro	Glu	Glu	Leu
Glu	Arg	Ala	Cys
Ser	Ile	His	Gly
Tyr	Ile	Glu	Thr
	Asn	Cys	Val
	Glu	Leu	Val
	Ile	Lys	Met
	Pro	Glu	Ala
	Asp	Leu	Thr
	Ile	Glu	Asp
	Asn	Val	Val
	Leu	Pro	Glu
	Asp	His	Lys
	Val	Phe	Ser
	Pro	His	Phe
	His	His	Asp
	Ser	Glu	Lys
	Tyr	Leu	Leu
	Ser	Val	Leu
	Val	Tyr	Lys
	Leu	Glu	Asp
	Glu	Ala	Lys
	Arg	Ile	Leu
	Phe	Ile	Pro
	Val	Met	Glu
	Glu	Val	Ala
	Leu	Val	Ala
	Cys	Leu	Leu
	Gly	Glu	Asp
	Phe	Ser	Thr
	Gln	Thr	Pro
	Ala	Gly	Arg
	Gly	Glu	Ala
	Ile	Ser	Pro
	Ile	Thr	Gln
	Ser	Phe	Gly
	Lys	Lys	Leu
	Gln	Met	Val
	Leu	Ile	Gln
	Arg	Leu	Phe
	Asp	Asp	Tle
	Leu	Leu	Ala
	Cys	Leu	Arg
	Pro	Lys	Ala
	Ser	Ser	Val
	Arg	Leu	Gly
	Gly	Trp	Ile
	Arg	Lys	Gly

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	359768	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.529	Depositor
Minimum map value	-0.221	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	446.88, 446.88, 446.88	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.064, 1.064, 1.064	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	Ln	0.16	0/231	0.42	0/294
2	S2	0.22	0/40843	0.35	1/63639 (0.0%)
3	SA	0.34	0/1778	0.57	0/2416
4	SB	0.21	0/1765	0.57	3/2362 (0.1%)
5	SD	0.20	0/1793	0.47	0/2414
6	SE	0.22	0/2118	0.46	0/2849
7	SF	0.21	0/1516	0.53	0/2037
8	SH	0.44	0/1519	0.70	0/2033
9	SI	0.21	0/1715	0.51	0/2287
10	SK	0.20	0/851	0.50	0/1147
11	SL	0.22	0/1268	0.45	0/1696
12	SP	0.19	0/1003	0.49	0/1342
13	SQ	0.41	0/1160	0.75	0/1553
14	SR	0.28	0/1105	0.58	0/1484
15	SS	0.35	0/1216	0.62	0/1628
16	ST	0.20	0/1131	0.49	0/1515
17	SU	0.21	0/831	0.53	0/1115
18	SV	0.22	0/643	0.56	0/860
19	SX	0.42	0/1116	0.63	1/1490 (0.1%)
20	Sa	0.24	0/836	0.54	0/1121
21	Sc	0.45	0/508	0.72	0/680
22	Sd	0.58	0/470	0.89	0/623
23	Sg	0.18	0/2493	0.50	0/3394
24	SC	0.24	0/1762	0.55	0/2381
25	SG	0.19	0/1946	0.51	0/2590
26	SJ	0.20	0/1550	0.44	0/2069
27	SM	0.15	0/950	0.46	0/1275
28	SN	0.20	0/1232	0.42	0/1656
29	SO	0.22	0/1062	0.53	2/1425 (0.1%)
30	SW	0.23	0/1051	0.45	0/1406
31	SY	0.23	0/1083	0.49	0/1438
32	SZ	0.59	0/604	0.98	1/810 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Sb	0.19	0/665	0.48	0/891
34	Se	0.19	0/465	0.43	0/612
35	Sf	0.20	0/560	0.57	0/745
36	CD	0.19	0/352	0.45	0/471
All	All	0.24	0/81191	0.45	8/117748 (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
22	Sd	0	1
26	SJ	0	1
31	SY	0	1
All	All	0	3

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	SB	150	ILE	N-CA-C	-6.50	102.97	110.05
4	SB	150	ILE	CA-C-N	5.92	132.84	121.54
4	SB	150	ILE	C-N-CA	5.92	132.84	121.54
29	SO	14	VAL	CA-C-N	5.33	131.28	121.70
29	SO	14	VAL	C-N-CA	5.33	131.28	121.70
2	S2	688	U	P-O3'-C3'	5.30	128.16	120.20
32	SZ	82	SER	N-CA-C	-5.29	107.00	113.50
19	SX	123	VAL	N-CA-C	-5.14	101.08	108.48

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	SJ	137	VAL	Peptide
31	SY	94	HIS	Peptide
22	Sd	37	ASN	Mainchain

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	Ln	230	0	276	4	0
2	S2	36538	0	18415	319	0
3	SA	1741	0	1746	24	0
4	SB	1738	0	1809	21	0
5	SD	1765	0	1865	28	0
6	SE	2076	0	2177	30	0
7	SF	1495	0	1549	21	0
8	SH	1497	0	1590	52	0
9	SI	1686	0	1772	22	0
10	SK	827	0	854	11	0
11	SL	1247	0	1323	20	0
12	SP	985	0	1031	12	0
13	SQ	1142	0	1213	20	0
14	SR	1090	0	1149	6	0
15	SS	1198	0	1261	25	0
16	ST	1112	0	1146	20	0
17	SU	821	0	883	10	0
18	SV	636	0	637	13	0
19	SX	1098	0	1167	12	0
20	Sa	821	0	870	19	0
21	Sc	506	0	536	9	0
22	Sd	459	0	448	7	0
23	Sg	2436	0	2393	53	0
24	SC	1725	0	1813	24	0
25	SG	1923	0	2088	35	0
26	SJ	1525	0	1640	12	0
27	SM	940	0	965	11	0
28	SN	1208	0	1294	14	0
29	SO	1049	0	1073	20	0
30	SW	1034	0	1080	12	0
31	SY	1065	0	1142	14	0
32	SZ	598	0	656	10	0
33	Sb	651	0	672	16	0
34	Se	459	0	503	5	0
35	Sf	548	0	552	10	0
36	CD	346	0	334	7	0
37	S2	21	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	SG	1	0	0	0	0
38	Sa	1	0	0	0	0
38	Sd	1	0	0	0	0
38	Sf	1	0	0	0	0
All	All	76240	0	59922	795	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (795) 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)
8:SH:8:ILE:HG21	8:SH:43:LEU:CD2	1.56	1.35
2:S2:533:A:H61	2:S2:550:C:N4	1.44	1.13
2:S2:1710:C:H42	2:S2:1823:A:N6	1.47	1.12
2:S2:533:A:N6	2:S2:550:C:H42	1.50	1.10
2:S2:1710:C:N4	2:S2:1823:A:H61	1.48	1.09
8:SH:8:ILE:HG21	8:SH:43:LEU:HD21	1.31	1.07
2:S2:886:A:N6	2:S2:901:G:C4	2.23	1.07
2:S2:140:C:N4	2:S2:313:A:H61	1.59	0.99
2:S2:140:C:H42	2:S2:313:A:N6	1.60	0.97
8:SH:11:PRO:HG2	8:SH:14:GLU:O	1.63	0.97
2:S2:1656:G:H1	2:S2:1668:U:H3	1.13	0.94
8:SH:8:ILE:HG21	8:SH:43:LEU:HD23	1.52	0.91
8:SH:9:VAL:HG12	8:SH:45:ILE:O	1.70	0.91
2:S2:1609:C:H42	2:S2:1630:A:H61	0.92	0.88
8:SH:8:ILE:CG2	8:SH:43:LEU:CD2	2.50	0.88
8:SH:19:PHE:HZ	8:SH:60:ILE:CG2	1.87	0.88
8:SH:6:ALA:HB1	8:SH:16:PRO:HG2	1.57	0.85
8:SH:19:PHE:CZ	8:SH:60:ILE:CG2	2.61	0.83
2:S2:1758:G:C6	2:S2:1771:G:N2	2.47	0.82
2:S2:925:G:H1	2:S2:1017:U:H3	1.31	0.78
8:SH:5:SER:N	8:SH:25:GLN:HG2	1.99	0.78
8:SH:8:ILE:HG21	8:SH:43:LEU:CG	2.14	0.78
2:S2:1758:G:O6	2:S2:1771:G:C2	2.38	0.76
8:SH:138:GLU:H	8:SH:159:ASP:HB2	1.50	0.76
2:S2:1729:U:H3	2:S2:1805:G:H1	1.30	0.75
2:S2:1609:C:H42	2:S2:1630:A:N6	1.77	0.75
8:SH:19:PHE:CZ	8:SH:60:ILE:HG21	2.23	0.74
2:S2:1752:C:N3	2:S2:1779:G:N1	2.36	0.73
8:SH:19:PHE:HZ	8:SH:60:ILE:HG21	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S2:533:A:H61	2:S2:550:C:H42	0.75	0.72
2:S2:886:A:N6	2:S2:901:G:C5	2.57	0.72
23:Sg:87:LEU:HD11	23:Sg:111:VAL:HG11	1.70	0.72
2:S2:1710:C:N3	2:S2:1823:A:N1	2.38	0.72
2:S2:140:C:N3	2:S2:313:A:N1	2.37	0.72
8:SH:8:ILE:CG2	8:SH:43:LEU:HG	2.20	0.71
2:S2:885:U:H3	2:S2:901:G:H1	1.36	0.71
23:Sg:157:SER:HB3	23:Sg:164:ILE:HG22	1.70	0.71
2:S2:748:C:H42	2:S2:795:A:N6	1.87	0.71
13:SQ:43:GLU:HB3	13:SQ:44:PRO:CD	2.21	0.70
2:S2:1609:C:N3	2:S2:1630:A:N1	2.39	0.70
13:SQ:48:GLN:C	13:SQ:50:LYS:H	1.98	0.69
2:S2:1024:A:OP2	28:SN:124:ARG:NH2	2.26	0.69
2:S2:1609:C:N4	2:S2:1630:A:H61	1.78	0.68
16:ST:85:ASN:HB2	16:ST:88:MET:HB2	1.75	0.68
19:SX:60:LYS:H	19:SX:114:ASP:HB2	1.60	0.67
32:SZ:54:THR:HA	32:SZ:57:LYS:HB3	1.78	0.66
8:SH:27:LEU:HD22	8:SH:43:LEU:HD11	1.76	0.66
8:SH:8:ILE:CG2	8:SH:43:LEU:O	2.43	0.66
2:S2:1017:U:H5'	28:SN:55:ARG:HE	1.61	0.66
8:SH:30:LEU:O	8:SH:34:SER:HB2	1.96	0.65
5:SD:123:LEU:HD11	5:SD:152:PHE:HB3	1.78	0.65
2:S2:1756:C:N4	2:S2:1775:U:N3	2.44	0.65
2:S2:140:C:H42	2:S2:313:A:H61	0.78	0.65
2:S2:1331:C:N4	36:CD:103:ARG:O	2.29	0.65
6:SE:97:GLU:OE1	6:SE:113:ARG:NH1	2.30	0.64
8:SH:8:ILE:HG22	8:SH:43:LEU:HG	1.77	0.64
25:SG:132:ARG:HG2	25:SG:133:LEU:H	1.63	0.64
31:SY:55:ILE:HG12	31:SY:75:ILE:HG12	1.79	0.64
2:S2:1776:G:N2	2:S2:1777:G:C6	2.65	0.64
18:SV:32:ILE:HG12	18:SV:60:ARG:HD2	1.78	0.64
8:SH:51:ILE:HD11	8:SH:176:VAL:HG12	1.80	0.64
2:S2:164:A:H3'	2:S2:165:G:H21	1.62	0.64
11:SL:4:ILE:HG23	11:SL:5:GLN:HG2	1.80	0.64
2:S2:1307:U:O2	35:Sf:135:HIS:NE2	2.31	0.64
5:SD:106:ARG:HG3	5:SD:175:VAL:HG22	1.80	0.64
2:S2:748:C:N4	2:S2:795:A:N6	2.45	0.63
2:S2:1488:C:O2'	2:S2:1490:G:OP2	2.14	0.63
2:S2:1091:C:HO2'	30:SW:2:VAL:N	1.96	0.63
3:SA:184:ARG:HB3	3:SA:191:ARG:HE	1.64	0.63
6:SE:122:LYS:NZ	6:SE:124:CYS:SG	2.72	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S2:1451:G:N7	14:SR:44:LYS:NZ	2.46	0.62
2:S2:1658:G:OP2	2:S2:1660:C:N4	2.31	0.62
23:Sg:272:GLN:NE2	23:Sg:284:PRO:O	2.32	0.62
25:SG:57:ASP:HB3	25:SG:98:ARG:HD2	1.80	0.62
4:SB:65:ARG:NH1	29:SO:51:GLU:OE1	2.28	0.62
7:SF:140:ASP:HB2	21:Sc:46:VAL:HG12	1.81	0.62
2:S2:1521:C:OP2	15:SS:136:THR:OG1	2.19	0.61
5:SD:94:ARG:NH1	36:CD:142:ASN:O	2.33	0.61
23:Sg:120:ILE:HB	23:Sg:132:TRP:HB2	1.83	0.61
31:SY:29:HIS:NE2	31:SY:69:THR:OG1	2.29	0.61
24:SC:72:ASP:OD2	24:SC:272:HIS:NE2	2.33	0.61
5:SD:172:VAL:HG22	5:SD:185:LYS:HG3	1.83	0.61
8:SH:19:PHE:CZ	8:SH:60:ILE:HG22	2.35	0.61
8:SH:30:LEU:HA	8:SH:34:SER:OG	2.01	0.61
2:S2:1494:U:H4'	2:S2:1495:G:H5''	1.82	0.60
2:S2:1543:U:OP1	13:SQ:37:ARG:NH2	2.33	0.60
19:SX:101:LEU:O	19:SX:123:VAL:HG13	2.01	0.60
2:S2:323:C:H2'	2:S2:327:G:H22	1.65	0.60
2:S2:1396:A:O2'	2:S2:1398:G:N7	2.33	0.60
6:SE:247:THR:HG22	6:SE:250:GLU:HG3	1.84	0.60
8:SH:24:SER:HA	8:SH:27:LEU:HD23	1.83	0.60
25:SG:70:HIS:O	25:SG:70:HIS:ND1	2.34	0.60
2:S2:77:A:N7	25:SG:154:ARG:NH1	2.49	0.60
25:SG:22:ARG:HH21	25:SG:25:ARG:HH12	1.49	0.60
2:S2:1254:C:O2'	17:SU:66:ARG:NH2	2.33	0.60
23:Sg:87:LEU:HB2	23:Sg:101:PHE:HB2	1.82	0.60
31:SY:52:PRO:HA	31:SY:55:ILE:HD12	1.83	0.60
2:S2:1:U:C2	2:S2:3:C:N4	2.70	0.60
7:SF:134:VAL:HG13	7:SF:135:ARG:HG2	1.83	0.59
23:Sg:297:THR:HG22	23:Sg:311:GLN:HG2	1.84	0.59
2:S2:991:G:N7	20:Sa:7:ASN:ND2	2.50	0.59
2:S2:563:G:H1	2:S2:592:C:H5	1.51	0.59
2:S2:168:C:O2	25:SG:132:ARG:NH1	2.35	0.59
2:S2:1228:A:H2'	2:S2:1229:G:C8	2.38	0.59
7:SF:126:THR:HA	7:SF:135:ARG:HE	1.67	0.59
2:S2:1752:C:C4	2:S2:1779:G:N2	2.71	0.58
2:S2:1854:U:OP1	29:SO:150:ARG:NH1	2.36	0.58
17:SU:22:ILE:HD11	17:SU:112:VAL:HG13	1.84	0.58
21:Sc:13:ARG:HB3	21:Sc:33:GLU:HG2	1.84	0.58
2:S2:1566:G:N7	16:ST:101:ARG:NH2	2.50	0.58
8:SH:8:ILE:HG23	8:SH:43:LEU:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:SG:186:GLN:OE1	25:SG:189:ARG:NH1	2.35	0.58
27:SM:55:ASN:HB2	27:SM:82:ASN:HB2	1.85	0.58
31:SY:112:ASN:HA	31:SY:115:LYS:HD3	1.85	0.58
18:SV:35:ASN:OD1	24:SC:267:GLN:NE2	2.36	0.58
19:SX:68:LYS:HB3	19:SX:91:LEU:HD22	1.85	0.58
2:S2:748:C:N4	2:S2:795:A:H61	2.00	0.58
7:SF:110:GLN:NE2	7:SF:114:ASN:OD1	2.35	0.58
8:SH:8:ILE:CG2	8:SH:43:LEU:CG	2.78	0.58
23:Sg:110:SER:HB2	23:Sg:153:CYS:HA	1.85	0.58
27:SM:66:GLU:HG3	27:SM:76:LEU:HD21	1.86	0.58
10:SK:1:MET:HE2	10:SK:47:LYS:HB2	1.86	0.58
4:SB:83:LYS:HD3	4:SB:106:THR:HG22	1.86	0.58
30:SW:80:ASP:OD1	30:SW:124:LYS:NZ	2.36	0.58
20:Sa:11:ALA:O	20:Sa:15:ARG:NH2	2.37	0.57
12:SP:18:ARG:NH1	15:SS:88:LYS:O	2.36	0.57
24:SC:146:GLU:HB3	24:SC:149:THR:HG22	1.86	0.57
2:S2:374:G:N2	11:SL:7:GLU:OE2	2.36	0.57
2:S2:1277:C:H2'	2:S2:1278:A:H8	1.69	0.57
5:SD:94:ARG:NH1	36:CD:142:ASN:OD1	2.36	0.57
11:SL:18:GLN:HG2	11:SL:33:LEU:HD11	1.85	0.57
18:SV:19:ALA:O	30:SW:23:ARG:NH1	2.32	0.57
3:SA:77:ILE:HG12	3:SA:99:ILE:HB	1.87	0.57
8:SH:8:ILE:HB	8:SH:27:LEU:HD21	1.87	0.57
21:Sc:24:GLN:OE1	21:Sc:26:GLN:NE2	2.37	0.57
2:S2:168:C:O2'	25:SG:133:LEU:O	2.22	0.57
2:S2:420:G:O2'	2:S2:660:C:N3	2.33	0.57
8:SH:8:ILE:CG2	8:SH:43:LEU:HD23	2.26	0.57
2:S2:1454:A:H5''	14:SR:3:ARG:HH11	1.70	0.57
3:SA:141:ASN:ND2	18:SV:31:SER:O	2.32	0.57
8:SH:8:ILE:HG13	8:SH:27:LEU:HD11	1.87	0.57
16:ST:76:THR:HG23	16:ST:94:ARG:HE	1.70	0.56
27:SM:52:LEU:HD11	27:SM:65:VAL:HG21	1.86	0.56
2:S2:1752:C:C2	2:S2:1779:G:N1	2.71	0.56
15:SS:81:ASP:O	15:SS:87:GLN:NE2	2.37	0.56
23:Sg:286:CYS:HA	23:Sg:302:TYR:HA	1.87	0.56
2:S2:1550:G:H3'	2:S2:1579:A:H61	1.71	0.56
4:SB:146:ARG:HB2	4:SB:149:GLN:HB2	1.87	0.56
12:SP:110:GLU:OE2	15:SS:116:LYS:NZ	2.39	0.56
2:S2:828:G:OP1	26:SJ:6:SER:OG	2.24	0.56
2:S2:1095:C:N3	2:S2:1149:A:N1	2.53	0.56
2:S2:1701:C:O2'	36:CD:103:ARG:NH1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S2:1764:G:H5'	2:S2:1765:C:H5''	1.88	0.56
2:S2:1860:A:H3'	20:Sa:8:ASN:HB3	1.87	0.56
2:S2:851:C:H5''	2:S2:852:G:H5'	1.87	0.56
2:S2:940:U:H3	2:S2:1002:U:H3	1.53	0.56
3:SA:36:GLN:O	3:SA:53:ARG:NH1	2.39	0.56
28:SN:87:ASP:HB3	28:SN:125:LEU:HD21	1.88	0.56
2:S2:1013:U:OP1	2:S2:1129:G:O2'	2.24	0.55
13:SQ:48:GLN:C	13:SQ:50:LYS:N	2.62	0.55
2:S2:962:A:H5''	29:SO:66:ARG:HG3	1.87	0.55
2:S2:1403:C:N4	2:S2:1433:C:OP1	2.39	0.55
1:Ln:11:ARG:NH2	2:S2:1184:G:OP1	2.39	0.55
2:S2:1758:G:C5	2:S2:1771:G:N2	2.75	0.55
2:S2:1292:C:N3	35:Sf:138:ARG:NH2	2.53	0.55
13:SQ:43:GLU:HB3	13:SQ:44:PRO:HD2	1.86	0.55
15:SS:118:ARG:HE	15:SS:123:LEU:HD21	1.71	0.55
23:Sg:99:ARG:HH22	23:Sg:136:GLY:HA3	1.71	0.55
29:SO:45:THR:OG1	29:SO:51:GLU:O	2.21	0.55
5:SD:74:GLN:NE2	5:SD:79:PHE:O	2.39	0.55
5:SD:137:VAL:HG22	5:SD:151:LYS:HG2	1.89	0.55
26:SJ:112:THR:HG22	26:SJ:123:ILE:HD11	1.88	0.55
2:S2:77:A:H62	25:SG:154:ARG:HH12	1.55	0.55
2:S2:507:G:OP1	31:SY:108:LYS:NZ	2.37	0.55
33:Sb:37:CYS:HB3	33:Sb:63:LEU:HD21	1.88	0.55
35:Sf:123:SER:OG	35:Sf:126:CYS:SG	2.65	0.55
2:S2:1755:C:C4	2:S2:1756:C:N4	2.75	0.55
2:S2:379:C:O2	9:SI:5:ARG:NH1	2.39	0.55
2:S2:749:U:O4	2:S2:793:G:N2	2.40	0.55
2:S2:1018:U:O2'	28:SN:86:GLU:OE2	2.24	0.55
2:S2:1536:G:H2'	2:S2:1537:A:C8	2.42	0.55
2:S2:1331:C:H41	36:CD:101:ASP:HA	1.72	0.54
11:SL:22:ARG:NH1	11:SL:23:VAL:O	2.39	0.54
15:SS:25:LYS:HD3	15:SS:55:ARG:HH11	1.71	0.54
2:S2:874:G:H2'	2:S2:875:A:H8	1.72	0.54
9:SI:139:LYS:HE2	9:SI:141:ARG:HH22	1.71	0.54
2:S2:1286:G:N7	27:SM:36:ARG:NE	2.55	0.54
2:S2:1536:G:H2'	2:S2:1537:A:H8	1.73	0.54
6:SE:11:ARG:HA	6:SE:28:ALA:HB2	1.89	0.54
16:ST:104:LEU:HD22	16:ST:121:ARG:HD2	1.89	0.54
2:S2:1589:A:N3	2:S2:1653:U:O2'	2.38	0.54
5:SD:64:ARG:NH2	10:SK:71:LEU:O	2.40	0.54
3:SA:187:GLY:HA2	18:SV:45:ARG:NH1	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:SF:28:VAL:O	7:SF:42:LYS:NZ	2.39	0.54
15:SS:72:GLN:HG3	15:SS:99:LEU:HD21	1.89	0.54
2:S2:1137:U:O3'	3:SA:155:ARG:NH2	2.41	0.54
6:SE:198:ARG:HG3	6:SE:208:VAL:HG12	1.89	0.54
2:S2:1756:C:N4	2:S2:1775:U:C4	2.76	0.53
5:SD:172:VAL:O	5:SD:173:ARG:NH1	2.39	0.53
24:SC:196:ILE:HB	24:SC:223:TYR:HB2	1.88	0.53
7:SF:142:SER:OG	21:Sc:49:PRO:O	2.22	0.53
11:SL:75:GLY:HA3	11:SL:88:ILE:HD12	1.90	0.53
20:Sa:59:PHE:HB2	20:Sa:62:TYR:HB2	1.90	0.53
1:Ln:17:ARG:NH1	2:S2:1173:A:OP1	2.41	0.53
2:S2:1723:G:H2'	2:S2:1724:A:C8	2.44	0.53
15:SS:124:ARG:HE	15:SS:129:LEU:HB2	1.73	0.53
2:S2:1485:U:OP1	5:SD:151:LYS:NZ	2.41	0.53
6:SE:45:ILE:HA	6:SE:61:VAL:HG11	1.89	0.53
8:SH:50:GLU:HG2	8:SH:60:ILE:HG22	1.90	0.53
9:SI:191:GLU:O	11:SL:19:ASN:ND2	2.42	0.53
28:SN:54:LEU:HB3	28:SN:60:VAL:HB	1.90	0.53
30:SW:3:ARG:HD3	30:SW:6:VAL:HG12	1.91	0.53
2:S2:416:U:HO2'	2:S2:652:U:HO2'	1.57	0.53
5:SD:177:LEU:O	5:SD:179:GLN:N	2.42	0.53
2:S2:1128:C:OP1	33:Sb:17:ARG:NH1	2.42	0.53
8:SH:58:LYS:HB2	8:SH:90:LYS:HG2	1.91	0.53
14:SR:27:ASP:O	14:SR:31:ASN:ND2	2.37	0.53
23:Sg:111:VAL:HG12	23:Sg:122:SER:HA	1.91	0.53
5:SD:8:LYS:HG2	17:SU:61:LEU:HD11	1.91	0.52
23:Sg:108:VAL:HA	23:Sg:124:SER:HA	1.91	0.52
8:SH:45:ILE:HD12	8:SH:62:ILE:HD12	1.91	0.52
2:S2:1154:U:OP2	24:SC:187:ARG:NH2	2.42	0.52
3:SA:108:PHE:HB3	3:SA:140:VAL:HG21	1.91	0.52
12:SP:81:ARG:NH1	12:SP:120:SER:OG	2.40	0.52
2:S2:167:G:O2'	25:SG:131:ARG:NH1	2.42	0.52
2:S2:317:C:OP2	25:SG:183:ARG:NH1	2.43	0.52
2:S2:880:G:O6	2:S2:906:U:O2	2.27	0.52
2:S2:156:G:OP1	25:SG:2:LYS:NZ	2.43	0.52
2:S2:928:G:H2'	2:S2:929:G:C8	2.44	0.52
21:Sc:12:ALA:HB1	21:Sc:32:VAL:HB	1.92	0.52
26:SJ:127:ARG:HD3	34:Se:31:ARG:HD3	1.92	0.52
2:S2:1436:C:O2'	2:S2:1438:A:OP2	2.28	0.52
2:S2:1597:C:H4'	2:S2:1603:G:C6	2.45	0.52
6:SE:44:LEU:HD13	6:SE:72:ILE:HD11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S2:1472:C:O3'	23:Sg:15:ASN:ND2	2.42	0.52
18:SV:71:ARG:HH11	33:Sb:4:ALA:HB2	1.75	0.52
2:S2:981:A:H2'	2:S2:982:G:C8	2.45	0.52
4:SB:40:ASN:ND2	4:SB:75:GLN:OE1	2.42	0.52
6:SE:185:GLY:H	6:SE:189:LEU:HD13	1.75	0.52
15:SS:68:ILE:HG23	15:SS:72:GLN:HE22	1.75	0.52
23:Sg:107:ASP:OD1	23:Sg:107:ASP:N	2.40	0.52
23:Sg:178:ASN:HB3	23:Sg:185:LYS:HE3	1.92	0.52
32:SZ:50:PHE:HB3	32:SZ:79:ILE:HD11	1.91	0.52
36:CD:119:GLY:HA3	36:CD:123:VAL:HG11	1.92	0.52
2:S2:1209:A:H5''	20:Sa:82:LYS:HE3	1.92	0.51
12:SP:64:LYS:NZ	12:SP:91:GLY:O	2.42	0.51
21:Sc:61:SER:OG	21:Sc:62:GLU:OE1	2.23	0.51
23:Sg:78:ALA:HB3	23:Sg:90:TRP:HB2	1.92	0.51
23:Sg:217:MET:HG2	23:Sg:229:THR:HG23	1.92	0.51
26:SJ:53:ILE:HD13	26:SJ:81:LEU:HD21	1.92	0.51
29:SO:45:THR:HA	29:SO:52:THR:HA	1.92	0.51
31:SY:110:ARG:HE	31:SY:128:GLY:HA3	1.75	0.51
7:SF:127:ARG:HG3	7:SF:136:ARG:HB2	1.91	0.51
28:SN:66:VAL:HG13	28:SN:67:THR:HG23	1.93	0.51
2:S2:1005:G:OP2	4:SB:162:ARG:NH2	2.40	0.51
16:ST:113:VAL:HG12	16:ST:123:LEU:HD23	1.92	0.51
25:SG:64:LYS:HB2	25:SG:97:VAL:HG11	1.92	0.51
27:SM:92:CYS:HB3	27:SM:94:ILE:HG12	1.92	0.51
2:S2:376:A:O3'	9:SI:99:ASN:ND2	2.44	0.51
2:S2:453:C:O2'	25:SG:92:ARG:O	2.22	0.51
3:SA:187:GLY:HA2	18:SV:45:ARG:HH11	1.75	0.51
8:SH:5:SER:HB3	8:SH:28:LEU:HD11	1.93	0.51
13:SQ:85:ARG:NH2	13:SQ:118:THR:OG1	2.43	0.51
4:SB:137:LEU:HG	4:SB:215:VAL:HG22	1.91	0.51
10:SK:65:ARG:NH2	22:Sd:21:CYS:O	2.44	0.51
13:SQ:48:GLN:HA	13:SQ:51:LEU:CD2	2.40	0.51
13:SQ:49:TYR:O	13:SQ:53:GLU:HG3	2.11	0.51
14:SR:16:ILE:HG22	14:SR:24:LEU:HD21	1.92	0.51
23:Sg:145:GLU:O	23:Sg:175:LYS:NZ	2.43	0.51
15:SS:16:LEU:HD21	15:SS:72:GLN:HE21	1.76	0.51
18:SV:30:ALA:O	18:SV:60:ARG:NH1	2.40	0.51
35:Sf:139:HIS:HB2	35:Sf:148:TYR:HB2	1.92	0.51
2:S2:1756:C:N4	2:S2:1775:U:H3	2.09	0.51
2:S2:1531:A:H4'	2:S2:1605:G:H4'	1.93	0.51
16:ST:9:VAL:O	16:ST:11:GLN:NE2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:SA:147:LEU:O	3:SA:165:ASN:ND2	2.39	0.50
25:SG:85:ARG:O	25:SG:87:ARG:NH1	2.44	0.50
35:Sf:138:ARG:HD2	35:Sf:147:THR:HG23	1.93	0.50
10:SK:73:ASN:O	10:SK:77:GLN:NE2	2.44	0.50
17:SU:51:LYS:HB2	17:SU:90:ASP:HB2	1.93	0.50
25:SG:134:GLY:HA3	25:SG:158:VAL:HG11	1.91	0.50
2:S2:1552:G:OP1	5:SD:9:ARG:NH2	2.43	0.50
3:SA:126:ASP:HB3	3:SA:129:ALA:HB3	1.93	0.50
29:SO:95:ILE:HB	29:SO:129:ILE:HG23	1.94	0.50
30:SW:24:GLN:HB2	33:Sb:7:LEU:HD13	1.93	0.50
31:SY:57:VAL:HB	31:SY:60:PHE:HE2	1.76	0.50
2:S2:28:U:H2'	2:S2:29:G:H8	1.75	0.50
2:S2:118:C:H1'	2:S2:445:A:C5	2.46	0.50
23:Sg:23:THR:HG22	23:Sg:31:ILE:HD12	1.92	0.50
2:S2:533:A:N1	2:S2:550:C:N3	2.59	0.50
2:S2:1374:C:O2'	2:S2:1464:C:O2	2.29	0.50
2:S2:107:A:H2'	2:S2:108:G:C8	2.47	0.50
2:S2:928:G:H1	2:S2:1013:U:H3	1.59	0.50
2:S2:993:G:OP1	2:S2:1131:G:N2	2.42	0.50
2:S2:1261:C:O2	22:Sd:10:HIS:NE2	2.41	0.50
3:SA:118:GLU:OE2	24:SC:65:LYS:N	2.44	0.50
13:SQ:112:LEU:HD22	13:SQ:119:LEU:HD13	1.93	0.50
4:SB:33:VAL:HG13	4:SB:44:ILE:HB	1.93	0.50
16:ST:85:ASN:ND2	16:ST:89:PRO:O	2.43	0.50
33:Sb:34:ASP:OD1	33:Sb:82:LYS:NZ	2.33	0.50
2:S2:913:A:H1'	8:SH:66:VAL:HB	1.94	0.50
9:SI:73:THR:O	9:SI:74:ARG:NH1	2.39	0.50
15:SS:98:VAL:HG11	15:SS:106:LYS:HG3	1.93	0.50
2:S2:433:A:H5''	9:SI:22:HIS:HB3	1.92	0.49
2:S2:1605:G:OP1	16:ST:84:ARG:NH2	2.45	0.49
23:Sg:176:VAL:HB	23:Sg:186:THR:HB	1.93	0.49
29:SO:14:VAL:H	29:SO:15:ILE:HA	1.77	0.49
33:Sb:36:LYS:N	33:Sb:78:SER:OG	2.42	0.49
2:S2:1060:A:H4'	2:S2:1061:U:H5'	1.94	0.49
13:SQ:116:ASP:OD1	13:SQ:118:THR:OG1	2.29	0.49
2:S2:71:G:H2'	2:S2:72:C:H4'	1.94	0.49
2:S2:329:G:H2'	2:S2:330:G:H8	1.77	0.49
8:SH:5:SER:N	8:SH:25:GLN:CG	2.72	0.49
15:SS:98:VAL:HG23	15:SS:103:LEU:HD12	1.93	0.49
23:Sg:208:ALA:HB3	23:Sg:239:LEU:HD21	1.93	0.49
25:SG:32:MET:HA	25:SG:52:ILE:HB	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:SW:60:LYS:NZ	33:Sb:23:ARG:O	2.46	0.49
2:S2:367:U:H4'	2:S2:371:A:C8	2.48	0.49
2:S2:1291:A:O2'	35:Sf:145:CYS:SG	2.66	0.49
4:SB:73:ASP:OD1	29:SO:128:ARG:NH2	2.40	0.49
24:SC:242:ASP:OD1	24:SC:246:LYS:NZ	2.45	0.49
30:SW:26:LEU:HB2	33:Sb:7:LEU:HD23	1.94	0.49
4:SB:138:PHE:O	4:SB:213:ARG:N	2.45	0.49
8:SH:19:PHE:HZ	8:SH:60:ILE:CB	2.26	0.49
9:SI:3:ILE:O	9:SI:30:GLY:N	2.40	0.49
2:S2:570:C:O2'	31:SY:34:THR:O	2.27	0.49
2:S2:641:A:O2'	2:S2:645:C:OP1	2.30	0.49
2:S2:830:A:OP2	2:S2:846:G:N2	2.46	0.49
2:S2:1228:A:H2'	2:S2:1229:G:H8	1.77	0.49
2:S2:1729:U:O4	2:S2:1805:G:O6	2.30	0.49
10:SK:80:ARG:HD3	10:SK:87:PRO:HA	1.94	0.49
29:SO:13:GLN:HB3	29:SO:15:ILE:HG13	1.94	0.49
15:SS:45:LEU:HD22	15:SS:50:ILE:HD11	1.95	0.49
21:Sc:20:ARG:HD2	21:Sc:28:THR:HB	1.94	0.49
2:S2:84:A:N3	2:S2:150:A:O2'	2.46	0.49
6:SE:115:THR:HG23	6:SE:118:GLU:H	1.78	0.49
4:SB:129:THR:HG23	4:SB:131:ASP:H	1.77	0.49
8:SH:11:PRO:CG	8:SH:14:GLU:O	2.48	0.49
25:SG:72:ARG:HD3	25:SG:96:SER:HB3	1.94	0.49
2:S2:1277:C:H2'	2:S2:1278:A:C8	2.48	0.48
14:SR:21:TYR:HE2	14:SR:61:ILE:HG21	1.76	0.48
23:Sg:88:ARG:HH11	23:Sg:97:THR:HG21	1.78	0.48
5:SD:50:ILE:HD11	5:SD:86:LEU:HD23	1.95	0.48
6:SE:124:CYS:HB3	6:SE:141:THR:HB	1.95	0.48
13:SQ:48:GLN:HA	13:SQ:51:LEU:HD23	1.96	0.48
33:Sb:49:HIS:HA	33:Sb:70:LYS:HA	1.95	0.48
2:S2:552:G:H2'	2:S2:553:U:C6	2.48	0.48
8:SH:79:LEU:HD22	8:SH:94:PHE:HZ	1.78	0.48
20:Sa:44:ILE:HG13	20:Sa:45:VAL:HG13	1.95	0.48
2:S2:43:U:OP2	2:S2:485:A:N6	2.45	0.48
2:S2:557:U:H2'	2:S2:558:G:C8	2.49	0.48
8:SH:129:ILE:HD11	8:SH:180:LEU:HD13	1.95	0.48
29:SO:53:ILE:HG23	29:SO:88:LEU:HD13	1.94	0.48
2:S2:860:G:H21	30:SW:107:SER:HB3	1.79	0.48
23:Sg:192:THR:OG1	23:Sg:213:ASP:OD2	2.31	0.48
2:S2:126:G:OP1	25:SG:198:ARG:NH1	2.36	0.48
2:S2:346:C:H5''	6:SE:38:LEU:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S2:1232:U:H2'	2:S2:1233:G:C8	2.48	0.48
23:Sg:70:VAL:HG11	23:Sg:112:ALA:HA	1.95	0.48
27:SM:20:GLU:HA	27:SM:23:LYS:HB2	1.95	0.48
2:S2:4:C:H4'	24:SC:207:ALA:HB2	1.96	0.48
2:S2:201:C:H5''	2:S2:202:G:H21	1.79	0.48
2:S2:840:C:H4'	2:S2:841:G:H5''	1.95	0.48
2:S2:1171:G:O2'	2:S2:1187:G:O6	2.30	0.48
2:S2:1220:A:N3	2:S2:1677:U:O2'	2.41	0.48
16:ST:108:GLU:OE2	16:ST:121:ARG:NH1	2.45	0.48
17:SU:46:LYS:HZ3	17:SU:97:ILE:HD11	1.79	0.48
36:CD:132:ASP:OD1	36:CD:132:ASP:N	2.44	0.48
23:Sg:32:LEU:HD21	23:Sg:71:ILE:HD11	1.95	0.48
23:Sg:198:VAL:HG12	23:Sg:209:SER:HA	1.96	0.48
25:SG:198:ARG:O	25:SG:202:ASN:ND2	2.46	0.48
1:Ln:1:MET:O	1:Ln:6:ARG:NH2	2.46	0.48
2:S2:35:C:H5''	2:S2:579:C:H5''	1.95	0.48
2:S2:1308:U:H2'	2:S2:1309:C:C6	2.48	0.48
23:Sg:20:GLN:O	23:Sg:34:ALA:N	2.46	0.48
2:S2:54:A:OP1	31:SY:111:LYS:NZ	2.38	0.48
2:S2:640:A:H2'	2:S2:641:A:C8	2.49	0.48
8:SH:51:ILE:HG21	8:SH:179:LYS:HG2	1.95	0.48
8:SH:160:LYS:HD3	8:SH:189:PHE:HB3	1.94	0.48
11:SL:29:GLY:HA3	11:SL:30:LYS:HA	1.61	0.48
11:SL:96:ILE:HD12	19:SX:10:ALA:HB1	1.96	0.48
23:Sg:152:SER:H	23:Sg:169:GLY:HA2	1.79	0.48
23:Sg:197:THR:OG1	23:Sg:237:ASN:O	2.31	0.48
29:SO:54:CYS:HB3	29:SO:84:ARG:HG2	1.96	0.48
2:S2:385:G:H3'	11:SL:136:LYS:HB2	1.96	0.47
11:SL:87:VAL:HA	11:SL:110:SER:HA	1.95	0.47
18:SV:3:ASN:HA	24:SC:173:LYS:HD3	1.96	0.47
23:Sg:256:ILE:HB	23:Sg:270:LEU:HB2	1.95	0.47
32:SZ:43:LYS:O	32:SZ:44:LEU:C	2.57	0.47
2:S2:885:U:O4	2:S2:901:G:O6	2.31	0.47
11:SL:73:LEU:HB3	11:SL:90:ARG:NH1	2.29	0.47
16:ST:114:GLU:OE2	16:ST:122:LYS:NZ	2.37	0.47
2:S2:959:G:OP1	29:SO:104:ARG:NH1	2.45	0.47
17:SU:21:ARG:HD3	17:SU:88:LEU:HD12	1.95	0.47
25:SG:148:SER:N	25:SG:151:ASP:OD2	2.47	0.47
2:S2:604:A:N3	2:S2:639:C:O2'	2.45	0.47
2:S2:902:G:O2'	2:S2:903:A:O4'	2.33	0.47
2:S2:944:A:H5''	29:SO:134:PRO:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S2:1144:A:H2'	2:S2:1145:A:C8	2.49	0.47
5:SD:45:ARG:HD2	5:SD:85:GLU:HG3	1.96	0.47
9:SI:190:LEU:HD22	9:SI:194:GLU:HG2	1.96	0.47
13:SQ:19:ALA:HB2	13:SQ:75:GLY:HA3	1.97	0.47
25:SG:135:PRO:HB2	25:SG:141:ILE:HG12	1.97	0.47
2:S2:987:A:C6	4:SB:120:MET:HE1	2.50	0.47
5:SD:56:GLN:NE2	5:SD:57:ASN:OD1	2.48	0.47
18:SV:80:SER:HB2	18:SV:83:PHE:HD1	1.80	0.47
19:SX:77:ASN:O	19:SX:79:LYS:N	2.44	0.47
20:Sa:32:LYS:O	20:Sa:37:LYS:NZ	2.39	0.47
2:S2:1752:C:O2	2:S2:1779:G:O6	2.32	0.47
10:SK:80:ARG:NH1	10:SK:89:ILE:O	2.47	0.47
15:SS:35:GLY:HA3	15:SS:99:LEU:HA	1.97	0.47
2:S2:750:C:H41	2:S2:793:G:H21	1.63	0.47
2:S2:1588:A:H2'	2:S2:1589:A:C8	2.50	0.47
6:SE:54:TYR:O	31:SY:15:ASN:ND2	2.47	0.47
7:SF:42:LYS:HG2	7:SF:43:GLU:HG2	1.97	0.47
15:SS:114:LEU:HA	15:SS:117:ILE:HG22	1.97	0.47
2:S2:846:G:H5''	6:SE:108:ARG:HH12	1.80	0.47
2:S2:948:C:H2'	2:S2:949:G:H8	1.80	0.47
2:S2:1752:C:N3	2:S2:1779:G:C2	2.82	0.47
7:SF:26:ASP:HA	7:SF:42:LYS:HG3	1.96	0.47
28:SN:130:LYS:NZ	28:SN:139:TRP:O	2.31	0.47
2:S2:448:A:H5''	9:SI:25:ARG:HA	1.96	0.47
2:S2:1726:G:C6	2:S2:1809:A:C6	3.03	0.47
2:S2:1147:C:OP1	20:Sa:6:ARG:NH1	2.48	0.46
2:S2:1854:U:H2'	2:S2:1855:G:H8	1.80	0.46
7:SF:25:THR:OG1	7:SF:26:ASP:N	2.48	0.46
8:SH:8:ILE:HG22	8:SH:43:LEU:O	2.15	0.46
8:SH:145:ARG:HD3	30:SW:51:GLU:HB2	1.97	0.46
12:SP:18:ARG:HD3	15:SS:88:LYS:HG2	1.96	0.46
32:SZ:84:ALA:O	32:SZ:88:LEU:HD23	2.15	0.46
2:S2:886:A:C6	2:S2:901:G:N3	2.83	0.46
2:S2:986:G:OP2	2:S2:988:C:N4	2.48	0.46
2:S2:1351:G:O2'	2:S2:1378:A:N1	2.47	0.46
2:S2:1512:C:H5''	22:Sd:8:TRP:HZ3	1.78	0.46
4:SB:134:LEU:HG	4:SB:218:LEU:HD12	1.97	0.46
6:SE:175:PHE:HE2	6:SE:198:ARG:HD2	1.79	0.46
23:Sg:199:THR:OG1	23:Sg:239:LEU:O	2.26	0.46
2:S2:1562:C:H2'	2:S2:1563:G:H8	1.80	0.46
5:SD:226:GLN:NE2	23:Sg:224:GLY:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S2:28:U:H2'	2:S2:29:G:C8	2.50	0.46
2:S2:1232:U:H2'	2:S2:1233:G:H8	1.79	0.46
8:SH:6:ALA:CB	8:SH:16:PRO:HG2	2.37	0.46
15:SS:36:VAL:HG21	15:SS:71:MET:HE3	1.97	0.46
23:Sg:11:LEU:HG	23:Sg:53:GLY:HA3	1.96	0.46
2:S2:391:C:H2'	2:S2:392:A:H8	1.80	0.46
2:S2:1289:U:H3	2:S2:1310:U:H3	1.62	0.46
2:S2:1714:U:H2'	2:S2:1715:A:C8	2.51	0.46
2:S2:1752:C:N4	2:S2:1779:G:N2	2.64	0.46
5:SD:140:GLY:HA3	5:SD:182:LEU:HD12	1.98	0.46
17:SU:56:MET:HE3	17:SU:88:LEU:HD21	1.97	0.46
31:SY:3:ASP:OD1	31:SY:3:ASP:N	2.49	0.46
2:S2:1723:G:H2'	2:S2:1724:A:H8	1.81	0.46
6:SE:79:ASP:HB3	6:SE:82:TYR:HB2	1.97	0.46
12:SP:25:LEU:HA	12:SP:28:MET:HE3	1.96	0.46
12:SP:49:LEU:HD21	12:SP:83:MET:HE1	1.98	0.46
2:S2:385:G:O2'	9:SI:10:LYS:NZ	2.43	0.46
2:S2:444:G:O6	9:SI:26:LYS:NZ	2.48	0.46
2:S2:847:A:O2'	6:SE:106:LYS:NZ	2.45	0.46
2:S2:907:G:H2'	2:S2:908:A:H8	1.80	0.46
6:SE:100:ARG:HH21	6:SE:118:GLU:HG2	1.80	0.46
6:SE:137:PRO:HB2	6:SE:150:PRO:HD2	1.98	0.46
6:SE:211:LYS:HE2	6:SE:215:GLY:HA2	1.98	0.46
10:SK:14:LEU:HD22	10:SK:35:LEU:HG	1.98	0.46
25:SG:181:THR:HG22	25:SG:184:VAL:HG23	1.97	0.46
32:SZ:47:LEU:HB3	32:SZ:79:ILE:HD12	1.98	0.46
2:S2:587:A:H5'	2:S2:592:C:H42	1.81	0.46
2:S2:912:C:O3'	8:SH:99:ARG:NH2	2.47	0.46
20:Sa:11:ALA:HB3	20:Sa:33:ASP:HB2	1.97	0.46
23:Sg:91:ASP:HB2	23:Sg:98:THR:HG23	1.97	0.46
2:S2:661:U:OP2	19:SX:3:LYS:NZ	2.49	0.46
2:S2:1010:G:H2'	2:S2:1011:A:C8	2.51	0.46
23:Sg:191:HIS:NE2	23:Sg:213:ASP:OD1	2.45	0.46
23:Sg:201:SER:OG	23:Sg:203:ASP:O	2.34	0.46
31:SY:12:PHE:HZ	31:SY:21:LYS:HD2	1.81	0.46
1:Ln:11:ARG:NH2	2:S2:1844:U:OP1	2.49	0.45
8:SH:95:ILE:HD11	8:SH:133:LEU:HD13	1.97	0.45
9:SI:104:ILE:O	9:SI:171:LEU:N	2.44	0.45
9:SI:141:ARG:HD3	9:SI:145:ILE:HG22	1.98	0.45
11:SL:39:ASN:C	11:SL:39:ASN:HD22	2.22	0.45
16:ST:65:TYR:HE1	16:ST:128:GLN:HG3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:SU:26:SER:HB2	17:SU:110:VAL:HG22	1.98	0.45
25:SG:20:ASP:OD1	25:SG:20:ASP:N	2.49	0.45
2:S2:1461:G:H3'	2:S2:1463:U:H3	1.81	0.45
2:S2:1636:G:O2'	7:SF:164:ARG:NH1	2.49	0.45
16:ST:56:ARG:HG3	16:ST:103:VAL:HG21	1.97	0.45
27:SM:23:LYS:HA	27:SM:23:LYS:HD3	1.79	0.45
28:SN:55:ARG:NH1	28:SN:56:ASP:OD1	2.48	0.45
2:S2:924:G:N2	28:SN:87:ASP:OD1	2.44	0.45
2:S2:928:G:N2	33:Sb:68:GLY:O	2.44	0.45
2:S2:886:A:N6	2:S2:901:G:N3	2.61	0.45
10:SK:90:VAL:HG13	10:SK:95:ARG:HD2	1.99	0.45
11:SL:28:THR:HA	11:SL:29:GLY:HA2	1.62	0.45
21:Sc:44:ARG:HA	21:Sc:44:ARG:HD2	1.82	0.45
2:S2:104:A:OP1	9:SI:12:ARG:NH1	2.46	0.45
23:Sg:72:SER:OG	23:Sg:74:ASP:OD1	2.30	0.45
2:S2:163:U:H2'	2:S2:164:A:H8	1.81	0.45
2:S2:1204:A:H5''	24:SC:117:ARG:HH11	1.82	0.45
2:S2:1421:A:H5''	2:S2:1422:G:C4	2.52	0.45
6:SE:66:MET:SD	6:SE:78:THR:OG1	2.75	0.45
6:SE:104:ASP:OD1	6:SE:105:THR:N	2.48	0.45
6:SE:197:ASN:ND2	6:SE:199:GLU:OE1	2.50	0.45
11:SL:3:ASP:OD1	11:SL:3:ASP:N	2.50	0.45
18:SV:27:LYS:HA	18:SV:27:LYS:HD3	1.83	0.45
24:SC:191:VAL:HG11	24:SC:236:PHE:HA	1.99	0.45
28:SN:25:TRP:CD2	33:Sb:82:LYS:HD3	2.52	0.45
5:SD:136:VAL:HG22	5:SD:186:VAL:HG23	1.98	0.45
2:S2:1:U:C2	2:S2:3:C:C4	3.05	0.45
2:S2:5:U:H2'	2:S2:6:G:H8	1.82	0.45
2:S2:155:G:H4'	25:SG:15:LEU:HD22	1.99	0.45
2:S2:795:A:H2'	2:S2:796:G:C8	2.51	0.45
2:S2:1354:G:N2	2:S2:1357:A:OP2	2.42	0.45
2:S2:145:G:H2'	2:S2:146:G:C8	2.52	0.44
13:SQ:86:GLN:HE22	13:SQ:122:ALA:HA	1.82	0.44
21:Sc:13:ARG:HH11	21:Sc:54:ASP:HA	1.82	0.44
29:SO:78:ALA:HB3	29:SO:118:ALA:HB3	1.97	0.44
33:Sb:36:LYS:HZ3	33:Sb:43:ILE:HA	1.82	0.44
2:S2:531:A:H3'	2:S2:532:C:H5''	1.99	0.44
2:S2:1780:G:O6	2:S2:1782:G:N2	2.51	0.44
2:S2:380:G:OP2	9:SI:181:GLN:NE2	2.47	0.44
2:S2:1203:G:H2'	2:S2:1204:A:C8	2.52	0.44
19:SX:134:TYR:O	34:Se:13:ARG:NH2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S2:309:G:OP2	9:SI:53:LYS:NZ	2.44	0.44
2:S2:329:G:H2'	2:S2:330:G:C8	2.53	0.44
2:S2:793:G:H2'	2:S2:794:A:C8	2.52	0.44
2:S2:1497:G:O6	10:SK:25:LYS:NZ	2.50	0.44
2:S2:1630:A:OP1	15:SS:40:TYR:N	2.47	0.44
4:SB:88:THR:OG1	4:SB:96:CYS:SG	2.66	0.44
15:SS:60:THR:OG1	15:SS:63:GLU:OE1	2.35	0.44
5:SD:110:LEU:HA	5:SD:177:LEU:HD21	1.98	0.44
8:SH:145:ARG:NH1	30:SW:51:GLU:OE1	2.48	0.44
9:SI:101:ILE:HD12	9:SI:190:LEU:HD11	1.99	0.44
23:Sg:40:ILE:HB	23:Sg:59:LEU:HB2	2.00	0.44
33:Sb:40:CYS:SG	33:Sb:41:TYR:N	2.90	0.44
2:S2:102:A:H4'	2:S2:104:A:C8	2.53	0.44
2:S2:990:A:H61	2:S2:1001:A:H61	1.66	0.44
2:S2:1217:A:H2'	2:S2:1218:C:C6	2.53	0.44
15:SS:17:ASN:HD21	15:SS:100:ALA:HB1	1.83	0.44
31:SY:118:ARG:HH11	31:SY:119:GLY:H	1.64	0.44
2:S2:57:U:OP1	2:S2:504:G:O2'	2.35	0.44
2:S2:1862:G:N2	20:Sa:76:SER:OG	2.41	0.44
20:Sa:43:ASN:HB3	20:Sa:45:VAL:HG22	1.99	0.44
24:SC:183:LYS:HG2	30:SW:95:PRO:HA	1.99	0.44
2:S2:1012:A:OP1	28:SN:3:ARG:NH1	2.43	0.44
2:S2:1174:U:H2'	2:S2:1175:G:H8	1.83	0.44
3:SA:118:GLU:HG3	24:SC:65:LYS:HD3	1.98	0.44
20:Sa:40:VAL:HG12	20:Sa:42:ARG:HG3	1.98	0.44
25:SG:2:LYS:HB2	25:SG:108:VAL:HG23	1.98	0.44
35:Sf:118:ARG:HB3	35:Sf:132:MET:HB3	1.99	0.44
35:Sf:132:MET:SD	35:Sf:139:HIS:HB3	2.58	0.44
2:S2:332:G:O6	25:SG:186:GLN:NE2	2.51	0.44
2:S2:1736:G:H2'	2:S2:1737:G:C8	2.52	0.44
2:S2:67:C:C5	25:SG:162:LEU:HB3	2.53	0.43
2:S2:220:U:H2'	2:S2:221:A:H8	1.83	0.43
2:S2:942:G:H2'	2:S2:943:U:C6	2.52	0.43
2:S2:956:G:O5'	29:SO:60:MET:HG2	2.17	0.43
2:S2:1098:C:H2'	2:S2:1099:G:C8	2.52	0.43
2:S2:1221:G:H2'	2:S2:1222:G:C8	2.52	0.43
2:S2:1644:C:H4'	13:SQ:140:ARG:HB2	2.00	0.43
2:S2:1861:G:H5''	20:Sa:3:LYS:HA	2.00	0.43
3:SA:41:ARG:HD2	3:SA:47:TYR:CZ	2.53	0.43
16:ST:56:ARG:HA	16:ST:56:ARG:HD3	1.79	0.43
2:S2:964:A:H2'	2:S2:965:U:H6	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S2:1679:A:N6	7:SF:58:ALA:O	2.51	0.43
17:SU:24:LEU:HD11	17:SU:39:LEU:HD12	1.99	0.43
23:Sg:24:THR:OG1	23:Sg:27:PHE:O	2.35	0.43
29:SO:57:THR:HG23	29:SO:60:MET:HE2	2.00	0.43
34:Se:12:VAL:HA	34:Se:15:GLN:HG2	2.00	0.43
2:S2:1613:G:OP1	15:SS:88:LYS:NZ	2.45	0.43
4:SB:125:VAL:HG22	4:SB:172:MET:HE3	1.99	0.43
6:SE:208:VAL:HG21	6:SE:225:ILE:HG13	2.00	0.43
16:ST:144:LYS:HD2	16:ST:144:LYS:HA	1.79	0.43
26:SJ:108:ARG:NH2	26:SJ:154:GLN:OE1	2.40	0.43
33:Sb:54:VAL:HG23	33:Sb:63:LEU:HB2	2.00	0.43
2:S2:1:U:O2	2:S2:3:C:C4	2.72	0.43
2:S2:589:G:N2	34:Se:23:GLU:OE2	2.52	0.43
2:S2:1139:C:H2'	2:S2:1140:G:O4'	2.17	0.43
8:SH:113:LYS:HD2	8:SH:113:LYS:HA	1.90	0.43
20:Sa:22:ARG:NH1	20:Sa:29:CYS:SG	2.91	0.43
27:SM:131:LYS:HG3	27:SM:132:LYS:HD3	2.01	0.43
2:S2:1726:G:N2	2:S2:1808:U:O2	2.52	0.43
35:Sf:124:ASP:N	35:Sf:124:ASP:OD1	2.50	0.43
2:S2:220:U:H2'	2:S2:221:A:C8	2.53	0.43
2:S2:1422:G:H1'	2:S2:1424:G:C8	2.53	0.43
3:SA:51:LEU:HA	3:SA:54:THR:HG22	2.01	0.43
15:SS:13:LEU:HB2	15:SS:20:ILE:HG12	2.00	0.43
20:Sa:23:CYS:O	29:SO:142:ARG:NH1	2.52	0.43
27:SM:53:ALA:O	27:SM:78:LYS:NZ	2.50	0.43
35:Sf:132:MET:HG3	35:Sf:133:ALA:H	1.84	0.43
2:S2:864:A:H2'	2:S2:865:A:H8	1.84	0.43
2:S2:1201:U:H2'	2:S2:1202:U:C6	2.54	0.43
2:S2:1660:C:H4'	2:S2:1663:A:H62	1.84	0.43
2:S2:1845:A:H2'	2:S2:1846:G:C8	2.53	0.43
11:SL:7:GLU:HG2	11:SL:8:ARG:H	1.84	0.43
11:SL:13:GLN:HE22	11:SL:63:THR:HB	1.84	0.43
16:ST:6:VAL:HG12	16:ST:135:ALA:HB2	2.01	0.43
29:SO:98:ARG:HH21	29:SO:134:PRO:HG2	1.84	0.43
2:S2:1189:A:H2'	2:S2:1190:A:C8	2.54	0.43
2:S2:1560:U:H2'	2:S2:1561:A:H8	1.84	0.43
2:S2:1628:C:H2'	2:S2:1629:C:C6	2.54	0.43
2:S2:1865:C:O2	20:Sa:92:ARG:HB3	2.19	0.43
7:SF:71:ARG:NH2	7:SF:148:ASN:OD1	2.35	0.43
8:SH:26:ALA:HB1	8:SH:86:LYS:HE3	2.00	0.43
2:S2:17:C:H2'	2:S2:18:C:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:SA:76:VAL:HG12	3:SA:123:VAL:HB	2.01	0.43
22:Sd:56:ASP:N	22:Sd:56:ASP:OD1	2.51	0.43
24:SC:113:GLN:HE21	24:SC:120:GLN:HG3	1.84	0.43
5:SD:158:ILE:HG13	5:SD:164:VAL:HG12	2.00	0.42
22:Sd:3:HIS:CE1	22:Sd:5:GLN:HB2	2.54	0.42
26:SJ:106:LEU:HD23	26:SJ:109:ARG:HD2	2.01	0.42
2:S2:1438:A:H2'	2:S2:1439:A:C8	2.54	0.42
5:SD:109:LEU:HD12	5:SD:184:ILE:HD11	2.01	0.42
9:SI:114:GLU:OE1	9:SI:114:GLU:N	2.52	0.42
33:Sb:46:VAL:HG11	33:Sb:54:VAL:HG21	2.00	0.42
2:S2:377:G:H5'	9:SI:98:LYS:HB3	2.02	0.42
2:S2:528:A:H2'	2:S2:529:A:H8	1.84	0.42
2:S2:649:U:H2'	2:S2:650:A:H8	1.84	0.42
2:S2:952:G:H2'	2:S2:953:C:C6	2.53	0.42
2:S2:1651:A:O2'	7:SF:83:ASN:OD1	2.27	0.42
2:S2:1695:A:N1	2:S2:1832:A:O2'	2.49	0.42
2:S2:1734:G:O2'	2:S2:1800:A:N6	2.51	0.42
3:SA:42:LYS:HD3	3:SA:46:ILE:HB	2.01	0.42
2:S2:466:G:H8	25:SG:59:GLN:HE21	1.67	0.42
2:S2:866:U:H2'	2:S2:867:G:C8	2.54	0.42
2:S2:988:C:H5''	4:SB:116:LYS:HG3	2.02	0.42
2:S2:1521:C:H1'	12:SP:128:HIS:HE1	1.85	0.42
11:SL:126:VAL:HG12	11:SL:145:VAL:HG22	1.99	0.42
2:S2:821:G:C6	26:SJ:150:ARG:HG3	2.54	0.42
2:S2:980:A:H2'	2:S2:981:A:C8	2.55	0.42
2:S2:1420:G:H21	2:S2:1421:A:H1'	1.84	0.42
3:SA:178:LEU:O	3:SA:182:VAL:HG23	2.19	0.42
9:SI:104:ILE:N	9:SI:171:LEU:O	2.47	0.42
20:Sa:13:LYS:HA	20:Sa:13:LYS:HD3	1.82	0.42
24:SC:110:MET:HA	24:SC:111:PRO:HD3	1.90	0.42
2:S2:115:U:H2'	2:S2:116:U:C6	2.54	0.42
2:S2:989:C:N4	2:S2:1001:A:C2	2.88	0.42
5:SD:175:VAL:HG12	5:SD:177:LEU:HG	2.01	0.42
24:SC:212:LYS:HD2	24:SC:212:LYS:HA	1.92	0.42
2:S2:533:A:N6	2:S2:550:C:N4	2.28	0.42
2:S2:833:C:H2'	2:S2:834:C:C6	2.54	0.42
2:S2:1295:A:N1	2:S2:1305:C:N4	2.67	0.42
2:S2:1736:G:H2'	2:S2:1737:G:H8	1.85	0.42
3:SA:34:MET:SD	3:SA:154:LEU:HD11	2.60	0.42
3:SA:220:LYS:HD3	3:SA:220:LYS:HA	1.81	0.42
4:SB:173:THR:O	4:SB:177:GLN:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:SB:178:THR:HG23	4:SB:179:ASN:ND2	2.35	0.42
2:S2:847:A:OP2	6:SE:16:LYS:NZ	2.46	0.42
24:SC:200:ARG:O	26:SJ:54:ARG:NH1	2.42	0.42
26:SJ:47:LYS:HB3	26:SJ:102:ILE:HD12	2.02	0.42
27:SM:75:ASN:ND2	27:SM:130:CYS:SG	2.81	0.42
28:SN:4:MET:HE3	28:SN:4:MET:HB2	1.98	0.42
2:S2:126:G:OP2	25:SG:195:LYS:NZ	2.36	0.42
2:S2:204:G:O2'	2:S2:205:G:O4'	2.35	0.42
2:S2:1213:C:H2'	2:S2:1214:A:C8	2.54	0.42
3:SA:69:GLU:HB2	24:SC:270:THR:HG21	2.02	0.42
4:SB:220:LYS:HA	4:SB:221:PRO:HD3	1.90	0.42
13:SQ:43:GLU:OE2	13:SQ:80:GLN:OE1	2.38	0.42
19:SX:6:GLY:O	19:SX:9:THR:OG1	2.29	0.42
23:Sg:17:TRP:HB2	23:Sg:36:ARG:HB2	2.02	0.42
23:Sg:227:LEU:HD23	23:Sg:227:LEU:HA	1.87	0.42
23:Sg:256:ILE:HD12	23:Sg:289:LEU:HD11	2.01	0.42
27:SM:126:GLU:HA	27:SM:129:LYS:HG2	2.02	0.42
2:S2:77:A:OP2	25:SG:155:GLN:NE2	2.52	0.42
2:S2:681:U:O2'	2:S2:1160:U:OP1	2.35	0.42
2:S2:1174:U:H2'	2:S2:1175:G:C8	2.54	0.42
11:SL:111:VAL:HG12	11:SL:140:PHE:HB2	2.02	0.42
18:SV:12:TYR:O	24:SC:248:TYR:OH	2.37	0.42
19:SX:39:ASN:HA	19:SX:40:PRO:HD3	1.90	0.42
19:SX:105:PHE:CD1	19:SX:121:LYS:HB3	2.55	0.42
20:Sa:22:ARG:NH2	29:SO:145:GLY:O	2.47	0.42
23:Sg:164:ILE:HD11	23:Sg:185:LYS:HD2	2.02	0.42
24:SC:278:THR:HA	24:SC:279:ARG:HA	1.64	0.42
28:SN:140:LYS:HD2	28:SN:140:LYS:HA	1.82	0.42
2:S2:5:U:H2'	2:S2:6:G:C8	2.54	0.41
2:S2:880:G:O6	2:S2:906:U:C2	2.73	0.41
3:SA:222:VAL:HG13	3:SA:223:THR:HG23	2.02	0.41
10:SK:53:LYS:HB3	10:SK:53:LYS:HE3	1.83	0.41
2:S2:748:C:N3	2:S2:795:A:N1	2.68	0.41
2:S2:996:A:H2'	2:S2:997:A:C8	2.55	0.41
4:SB:179:ASN:OD1	4:SB:187:LYS:NZ	2.37	0.41
8:SH:101:LEU:HD13	8:SH:120:ARG:HG2	2.02	0.41
9:SI:53:LYS:HB2	9:SI:53:LYS:HE3	1.79	0.41
24:SC:130:ILE:HD13	24:SC:159:LYS:HG3	2.01	0.41
32:SZ:57:LYS:NZ	32:SZ:61:GLU:OE2	2.42	0.41
32:SZ:78:LYS:HD2	32:SZ:78:LYS:HA	1.92	0.41
2:S2:441:C:H2'	2:S2:442:C:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S2:880:G:H3'	2:S2:881:G:H8	1.84	0.41
2:S2:1513:C:H2'	2:S2:1514:G:H8	1.86	0.41
7:SF:70:GLU:OE2	7:SF:86:LYS:NZ	2.37	0.41
7:SF:78:MET:HE3	7:SF:78:MET:HB2	1.98	0.41
25:SG:23:LYS:O	25:SG:26:THR:OG1	2.33	0.41
32:SZ:41:ARG:HD2	32:SZ:41:ARG:HA	1.83	0.41
2:S2:16:G:H2'	2:S2:17:C:C6	2.55	0.41
2:S2:51:U:H2'	2:S2:52:G:C8	2.55	0.41
2:S2:604:A:H5''	26:SJ:22:LYS:HE3	2.01	0.41
4:SB:37:ALA:HA	4:SB:42:ARG:HD3	2.02	0.41
5:SD:220:THR:OG1	5:SD:221:THR:N	2.53	0.41
18:SV:12:TYR:CD1	24:SC:79:GLU:HB2	2.55	0.41
23:Sg:79:LEU:HD22	23:Sg:120:ILE:HD12	2.02	0.41
2:S2:929:G:H2'	2:S2:930:C:O4'	2.20	0.41
6:SE:18:TRP:HH2	6:SE:31:PRO:HD3	1.85	0.41
7:SF:87:LEU:HD11	13:SQ:47:LEU:HG	2.03	0.41
11:SL:32:LYS:HA	11:SL:32:LYS:HD3	1.92	0.41
11:SL:39:ASN:O	11:SL:39:ASN:ND2	2.45	0.41
15:SS:70:ILE:HG12	15:SS:77:TYR:CD2	2.55	0.41
15:SS:75:ARG:HD3	15:SS:95:TYR:HB2	2.01	0.41
2:S2:538:U:H2'	2:S2:539:C:C6	2.56	0.41
2:S2:1190:A:N3	2:S2:1714:U:O2'	2.46	0.41
2:S2:1726:G:C6	2:S2:1809:A:N1	2.88	0.41
2:S2:1797:U:H2'	2:S2:1798:C:C6	2.56	0.41
5:SD:141:LYS:NZ	5:SD:179:GLN:O	2.43	0.41
10:SK:47:LYS:HA	10:SK:47:LYS:HD3	1.86	0.41
19:SX:47:ALA:O	19:SX:102:VAL:N	2.54	0.41
26:SJ:113:GLN:OE1	26:SJ:154:GLN:NE2	2.44	0.41
26:SJ:137:VAL:HG12	26:SJ:138:ARG:H	1.85	0.41
2:S2:649:U:H2'	2:S2:650:A:C8	2.55	0.41
2:S2:1221:G:H2'	2:S2:1222:G:H8	1.86	0.41
8:SH:157:HIS:HB3	8:SH:190:PRO:HG3	2.03	0.41
16:ST:39:LEU:HA	16:ST:39:LEU:HD12	1.83	0.41
16:ST:42:HIS:HB3	16:ST:93:SER:HB3	2.02	0.41
2:S2:414:A:OP1	2:S2:814:U:O2'	2.38	0.41
6:SE:107:GLY:HA2	6:SE:189:LEU:HG	2.01	0.41
17:SU:66:ARG:HG3	17:SU:68:THR:HG22	2.01	0.41
2:S2:29:G:H2'	2:S2:30:C:C6	2.55	0.41
2:S2:51:U:H2'	2:S2:52:G:H8	1.86	0.41
2:S2:1025:U:OP1	2:S2:1090:C:O2'	2.37	0.41
2:S2:1037:G:H4'	2:S2:1845:A:H4'	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S2:1320:G:H2'	2:S2:1321:G:O4'	2.21	0.41
2:S2:1475:G:H5'	13:SQ:124:PRO:HG3	2.03	0.41
2:S2:1648:G:O2'	2:S2:1674:G:O6	2.34	0.41
3:SA:206:ASP:HA	3:SA:207:PRO:HD3	1.95	0.41
5:SD:7:LYS:HD3	5:SD:7:LYS:HA	1.86	0.41
5:SD:141:LYS:HB3	5:SD:141:LYS:HE3	1.89	0.41
8:SH:81:ARG:HA	8:SH:84:GLU:HB2	2.03	0.41
13:SQ:8:GLN:O	13:SQ:26:LYS:HA	2.21	0.41
23:Sg:37:ASP:OD1	23:Sg:37:ASP:N	2.53	0.41
24:SC:271:ASP:N	24:SC:271:ASP:OD1	2.49	0.41
25:SG:2:LYS:H	25:SG:2:LYS:HG2	1.72	0.41
30:SW:3:ARG:HH22	30:SW:28:ARG:HH21	1.69	0.41
33:Sb:63:LEU:HD23	33:Sb:63:LEU:HA	1.94	0.41
2:S2:613:G:N2	2:S2:626:G:OP1	2.41	0.41
2:S2:1025:U:H2'	2:S2:1026:C:O4'	2.21	0.41
2:S2:1568:C:OP1	16:ST:96:SER:OG	2.36	0.41
2:S2:1568:C:H2'	2:S2:1569:A:C8	2.56	0.41
6:SE:45:ILE:HG13	6:SE:61:VAL:HG21	2.02	0.41
7:SF:68:ILE:HD12	7:SF:68:ILE:HA	1.95	0.41
16:ST:134:ILE:HG13	16:ST:137:GLN:NE2	2.36	0.41
23:Sg:5:MET:HB2	23:Sg:270:LEU:HD21	2.03	0.41
23:Sg:20:GLN:HB3	23:Sg:34:ALA:HB3	2.03	0.41
23:Sg:78:ALA:O	23:Sg:90:TRP:N	2.46	0.41
23:Sg:141:THR:OG1	23:Sg:142:VAL:N	2.54	0.41
2:S2:1130:G:H4'	28:SN:10:GLY:HA2	2.03	0.40
2:S2:1784:G:H2'	2:S2:1785:C:C6	2.56	0.40
3:SA:206:ASP:N	3:SA:206:ASP:OD1	2.51	0.40
6:SE:41:CYS:HA	6:SE:85:GLY:HA2	2.03	0.40
23:Sg:99:ARG:NH2	23:Sg:136:GLY:HA3	2.36	0.40
24:SC:168:GLY:N	24:SC:179:THR:O	2.37	0.40
2:S2:582:U:H1'	31:SY:33:ALA:HB2	2.03	0.40
2:S2:1496:U:H4'	22:Sd:24:CYS:HB2	2.02	0.40
6:SE:88:ASP:OD1	6:SE:122:LYS:HE3	2.22	0.40
7:SF:118:ASN:ND2	7:SF:181:ALA:O	2.54	0.40
23:Sg:10:THR:HG23	23:Sg:308:ARG:HD3	2.02	0.40
25:SG:147:LEU:HB3	25:SG:151:ASP:HB2	2.03	0.40
32:SZ:62:VAL:HA	32:SZ:65:TYR:CZ	2.57	0.40
32:SZ:99:LEU:HD21	32:SZ:102:LYS:HB2	2.02	0.40
2:S2:178:C:H2'	2:S2:179:C:H6	1.86	0.40
2:S2:553:U:H2'	2:S2:554:A:C8	2.57	0.40
2:S2:595:U:H2'	2:S2:596:U:C6	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S2:1240:A:C6	12:SP:100:LYS:HB2	2.57	0.40
2:S2:1420:G:N2	2:S2:1421:A:N3	2.66	0.40
2:S2:1617:G:H4'	22:Sd:14:PHE:CZ	2.56	0.40
2:S2:1622:U:OP1	15:SS:120:HIS:ND1	2.43	0.40
2:S2:1710:C:H42	2:S2:1823:A:H61	0.65	0.40
5:SD:185:LYS:HE3	5:SD:185:LYS:HB2	1.85	0.40
6:SE:51:ARG:NH1	6:SE:109:PHE:O	2.53	0.40
20:Sa:64:LEU:HA	20:Sa:65:PRO:HD3	1.90	0.40
29:SO:95:ILE:HG21	29:SO:116:LEU:HD11	2.03	0.40
2:S2:65:C:N3	25:SG:133:LEU:HB3	2.36	0.40
2:S2:900:C:H5'	2:S2:901:G:N7	2.36	0.40
2:S2:1716:C:H2'	2:S2:1717:C:H6	1.86	0.40
4:SB:65:ARG:HB3	4:SB:88:THR:HG22	2.03	0.40
7:SF:48:TYR:HB3	13:SQ:49:TYR:HB3	2.02	0.40
12:SP:33:LEU:HD12	12:SP:33:LEU:HA	1.92	0.40
12:SP:83:MET:HB3	12:SP:116:LEU:HD22	2.03	0.40
19:SX:71:ARG:NH1	19:SX:82:THR:OG1	2.48	0.40
23:Sg:168:CYS:HB2	23:Sg:195:LEU:HD22	2.03	0.40
23:Sg:252:THR:HG21	23:Sg:257:LYS:HE2	2.03	0.40
2:S2:1521:C:H1'	12:SP:128:HIS:CE1	2.57	0.40
2:S2:1543:U:OP2	16:ST:62:ARG:NH2	2.43	0.40
3:SA:89:LYS:HD3	14:SR:78:ARG:HH22	1.86	0.40
7:SF:193:LYS:NZ	7:SF:197:GLU:OE2	2.55	0.40
8:SH:130:LEU:HD21	8:SH:156:VAL:HG21	2.03	0.40
9:SI:172:LEU:HD23	9:SI:172:LEU:HA	1.87	0.40
13:SQ:48:GLN:O	13:SQ:50:LYS:N	2.55	0.40
23:Sg:65:PHE:O	23:Sg:83:TRP:N	2.38	0.40
34:Se:29:THR:HA	34:Se:33:LYS: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	
1	Ln	22/25 (88%)	22 (100%)	0	0	100	100
3	SA	219/295 (74%)	210 (96%)	8 (4%)	1 (0%)	24	54
4	SB	212/264 (80%)	195 (92%)	15 (7%)	2 (1%)	14	41
5	SD	225/243 (93%)	214 (95%)	10 (4%)	1 (0%)	30	59
6	SE	260/263 (99%)	253 (97%)	7 (3%)	0	100	100
7	SF	187/204 (92%)	172 (92%)	14 (8%)	1 (0%)	24	54
8	SH	182/194 (94%)	158 (87%)	22 (12%)	2 (1%)	11	36
9	SI	204/208 (98%)	189 (93%)	14 (7%)	1 (0%)	24	54
10	SK	96/165 (58%)	89 (93%)	7 (7%)	0	100	100
11	SL	151/158 (96%)	144 (95%)	7 (5%)	0	100	100
12	SP	119/145 (82%)	115 (97%)	4 (3%)	0	100	100
13	SQ	142/146 (97%)	133 (94%)	6 (4%)	3 (2%)	5	21
14	SR	133/135 (98%)	125 (94%)	7 (5%)	1 (1%)	16	44
15	SS	143/152 (94%)	134 (94%)	9 (6%)	0	100	100
16	ST	141/145 (97%)	132 (94%)	9 (6%)	0	100	100
17	SU	102/119 (86%)	95 (93%)	7 (7%)	0	100	100
18	SV	81/83 (98%)	74 (91%)	7 (9%)	0	100	100
19	SX	139/143 (97%)	132 (95%)	6 (4%)	1 (1%)	18	48
20	Sa	100/115 (87%)	93 (93%)	6 (6%)	1 (1%)	12	39
21	Sc	62/69 (90%)	51 (82%)	9 (14%)	2 (3%)	3	13
22	Sd	53/56 (95%)	47 (89%)	6 (11%)	0	100	100
23	Sg	311/317 (98%)	278 (89%)	33 (11%)	0	100	100
24	SC	220/293 (75%)	208 (94%)	12 (6%)	0	100	100
25	SG	235/249 (94%)	222 (94%)	12 (5%)	1 (0%)	30	59
26	SJ	183/194 (94%)	176 (96%)	7 (4%)	0	100	100
27	SM	120/132 (91%)	117 (98%)	3 (2%)	0	100	100
28	SN	148/151 (98%)	143 (97%)	5 (3%)	0	100	100
29	SO	138/151 (91%)	130 (94%)	7 (5%)	1 (1%)	18	48
30	SW	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
31	SY	129/133 (97%)	123 (95%)	6 (5%)	0	100	100
32	SZ	73/125 (58%)	58 (80%)	11 (15%)	4 (6%)	1	4
33	Sb	81/84 (96%)	72 (89%)	9 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	Se	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
35	Sf	65/156 (42%)	60 (92%)	5 (8%)	0	100	100
36	CD	44/469 (9%)	40 (91%)	4 (9%)	0	100	100
All	All	4903/5970 (82%)	4579 (93%)	302 (6%)	22 (0%)	31	59

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	SD	178	ARG
9	SI	160	SER
13	SQ	6	PRO
8	SH	45	ILE
13	SQ	43	GLU
13	SQ	49	TYR
21	Sc	36	ASP
32	SZ	78	LYS
4	SB	222	LYS
14	SR	129	LYS
19	SX	124	LYS
32	SZ	49	LEU
3	SA	11	LYS
7	SF	58	ALA
21	Sc	34	PHE
25	SG	13	GLN
4	SB	151	ARG
29	SO	140	THR
32	SZ	42	ASP
32	SZ	80	ARG
20	Sa	47	ALA
8	SH	8	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Ln	23/24 (96%)	23 (100%)	0	100	100
3	SA	183/243 (75%)	183 (100%)	0	100	100
4	SB	195/231 (84%)	195 (100%)	0	100	100
5	SD	190/202 (94%)	190 (100%)	0	100	100
6	SE	224/225 (100%)	224 (100%)	0	100	100
7	SF	159/170 (94%)	159 (100%)	0	100	100
8	SH	166/174 (95%)	161 (97%)	5 (3%)	36	70
9	SI	178/180 (99%)	178 (100%)	0	100	100
10	SK	89/136 (65%)	89 (100%)	0	100	100
11	SL	137/142 (96%)	136 (99%)	1 (1%)	76	92
12	SP	107/130 (82%)	107 (100%)	0	100	100
13	SQ	119/121 (98%)	112 (94%)	7 (6%)	18	48
14	SR	122/122 (100%)	122 (100%)	0	100	100
15	SS	126/132 (96%)	125 (99%)	1 (1%)	73	90
16	ST	113/115 (98%)	113 (100%)	0	100	100
17	SU	94/107 (88%)	94 (100%)	0	100	100
18	SV	67/67 (100%)	67 (100%)	0	100	100
19	SX	113/115 (98%)	111 (98%)	2 (2%)	51	80
20	Sa	89/98 (91%)	89 (100%)	0	100	100
21	Sc	57/62 (92%)	57 (100%)	0	100	100
22	Sd	48/49 (98%)	46 (96%)	2 (4%)	26	60
23	Sg	272/275 (99%)	272 (100%)	0	100	100
24	SC	188/225 (84%)	188 (100%)	0	100	100
25	SG	207/218 (95%)	207 (100%)	0	100	100
26	SJ	161/168 (96%)	161 (100%)	0	100	100
27	SM	102/108 (94%)	102 (100%)	0	100	100
28	SN	130/131 (99%)	130 (100%)	0	100	100
29	SO	110/119 (92%)	110 (100%)	0	100	100
30	SW	112/113 (99%)	112 (100%)	0	100	100
31	SY	113/115 (98%)	113 (100%)	0	100	100
32	SZ	66/103 (64%)	59 (89%)	7 (11%)	6	22
33	Sb	75/76 (99%)	75 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	Se	47/48 (98%)	47 (100%)	0	100	100
35	Sf	60/140 (43%)	60 (100%)	0	100	100
36	CD	35/404 (9%)	35 (100%)	0	100	100
All	All	4277/5088 (84%)	4252 (99%)	25 (1%)	76	93

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	SH	9	VAL
8	SH	27	LEU
8	SH	29	GLU
8	SH	41	ARG
8	SH	43	LEU
11	SL	39	ASN
13	SQ	10	VAL
13	SQ	39	LEU
13	SQ	41	MET
13	SQ	42	ILE
13	SQ	46	THR
13	SQ	48	GLN
13	SQ	100	VAL
15	SS	5	ILE
19	SX	123	VAL
19	SX	125	VAL
22	Sd	26	ASN
22	Sd	27	ARG
32	SZ	42	ASP
32	SZ	44	LEU
32	SZ	50	PHE
32	SZ	51	ASP
32	SZ	75	GLU
32	SZ	79	ILE
32	SZ	83	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	Ln	22	GLN
3	SA	9	GLN
4	SB	40	ASN

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Mol	Chain	Res	Type
4	SB	92	GLN
4	SB	101	HIS
4	SB	149	GLN
4	SB	202	GLN
5	SD	56	GLN
5	SD	101	GLN
6	SE	67	GLN
6	SE	179	ASN
6	SE	197	ASN
7	SF	31	ASN
7	SF	82	ASN
8	SH	12	ASN
8	SH	25	GLN
8	SH	112	ASN
8	SH	162	GLN
9	SI	52	ASN
9	SI	146	GLN
10	SK	7	ASN
10	SK	28	HIS
11	SL	39	ASN
11	SL	94	HIS
12	SP	128	HIS
13	SQ	97	GLN
14	SR	116	ASN
15	SS	10	GLN
15	SS	72	GLN
15	SS	87	GLN
16	ST	51	ASN
17	SU	81	GLN
19	SX	39	ASN
19	SX	61	GLN
20	Sa	19	GLN
20	Sa	25	ASN
21	Sc	26	GLN
21	Sc	29	GLN
22	Sd	3	HIS
22	Sd	5	GLN
23	Sg	20	GLN
23	Sg	119	GLN
23	Sg	226	HIS
24	SC	136	HIS
27	SM	82	ASN

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Mol	Chain	Res	Type
28	SN	58	HIS
29	SO	83	GLN
30	SW	91	ASN
32	SZ	45	ASN
32	SZ	106	GLN
32	SZ	112	ASN
33	Sb	65	GLN
33	Sb	84	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	S2	1699/1869 (90%)	376 (22%)	4 (0%)

All (376) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	S2	4	C
2	S2	14	C
2	S2	33	G
2	S2	41	G
2	S2	45	A
2	S2	46	A
2	S2	56	G
2	S2	58	C
2	S2	59	U
2	S2	62	G
2	S2	64	A
2	S2	65	C
2	S2	67	C
2	S2	68	A
2	S2	72	C
2	S2	73	C
2	S2	74	G
2	S2	76	U
2	S2	92	A
2	S2	103	A
2	S2	113	G
2	S2	114	G
2	S2	115	U
2	S2	126	G

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Mol	Chain	Res	Type
2	S2	127	C
2	S2	143	U
2	S2	149	A
2	S2	162	C
2	S2	170	A
2	S2	173	A
2	S2	182	C
2	S2	184	G
2	S2	196	C
2	S2	197	U
2	S2	198	U
2	S2	199	C
2	S2	200	G
2	S2	202	G
2	S2	203	G
2	S2	204	G
2	S2	207	G
2	S2	213	G
2	S2	224	A
2	S2	291	G
2	S2	292	A
2	S2	293	C
2	S2	295	C
2	S2	306	C
2	S2	308	G
2	S2	309	G
2	S2	312	G
2	S2	314	U
2	S2	319	C
2	S2	323	C
2	S2	324	C
2	S2	325	C
2	S2	326	C
2	S2	328	U
2	S2	329	G
2	S2	332	G
2	S2	347	G
2	S2	351	G
2	S2	361	U
2	S2	362	C
2	S2	364	A
2	S2	368	U

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Mol	Chain	Res	Type
2	S2	369	C
2	S2	370	G
2	S2	381	C
2	S2	385	G
2	S2	386	C
2	S2	409	C
2	S2	413	G
2	S2	421	G
2	S2	429	C
2	S2	441	C
2	S2	448	A
2	S2	449	A
2	S2	450	C
2	S2	452	G
2	S2	464	A
2	S2	465	A
2	S2	471	G
2	S2	472	C
2	S2	473	A
2	S2	474	G
2	S2	482	G
2	S2	487	U
2	S2	488	U
2	S2	492	C
2	S2	502	C
2	S2	508	A
2	S2	516	A
2	S2	523	A
2	S2	525	A
2	S2	528	A
2	S2	529	A
2	S2	531	A
2	S2	532	C
2	S2	534	G
2	S2	536	A
2	S2	537	C
2	S2	538	U
2	S2	540	U
2	S2	542	U
2	S2	546	G
2	S2	547	G
2	S2	548	C

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Mol	Chain	Res	Type
2	S2	555	A
2	S2	556	U
2	S2	557	U
2	S2	558	G
2	S2	563	G
2	S2	564	A
2	S2	570	C
2	S2	576	A
2	S2	583	A
2	S2	587	A
2	S2	589	G
2	S2	590	A
2	S2	591	U
2	S2	593	C
2	S2	594	A
2	S2	596	U
2	S2	597	G
2	S2	605	A
2	S2	606	G
2	S2	614	C
2	S2	617	G
2	S2	622	C
2	S2	623	G
2	S2	629	A
2	S2	632	C
2	S2	643	A
2	S2	644	G
2	S2	655	A
2	S2	660	C
2	S2	664	A
2	S2	666	U
2	S2	668	A
2	S2	669	A
2	S2	671	A
2	S2	672	A
2	S2	673	G
2	S2	683	G
2	S2	687	C
2	S2	688	U
2	S2	689	U
2	S2	749	U
2	S2	751	G

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Mol	Chain	Res	Type
2	S2	752	G
2	S2	788	G
2	S2	791	C
2	S2	792	C
2	S2	794	A
2	S2	797	C
2	S2	798	G
2	S2	799	U
2	S2	801	U
2	S2	811	A
2	S2	821	G
2	S2	822	U
2	S2	823	U
2	S2	824	C
2	S2	830	A
2	S2	836	G
2	S2	837	A
2	S2	838	G
2	S2	839	C
2	S2	841	G
2	S2	842	C
2	S2	847	A
2	S2	870	A
2	S2	874	G
2	S2	877	C
2	S2	878	G
2	S2	880	G
2	S2	883	U
2	S2	885	U
2	S2	888	U
2	S2	889	U
2	S2	891	G
2	S2	896	U
2	S2	897	U
2	S2	898	U
2	S2	899	U
2	S2	900	C
2	S2	901	G
2	S2	903	A
2	S2	904	A
2	S2	913	A
2	S2	914	U

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Mol	Chain	Res	Type
2	S2	920	A
2	S2	922	A
2	S2	930	C
2	S2	933	G
2	S2	934	G
2	S2	943	U
2	S2	955	A
2	S2	956	G
2	S2	963	A
2	S2	970	G
2	S2	971	G
2	S2	972	A
2	S2	990	A
2	S2	992	A
2	S2	999	G
2	S2	1001	A
2	S2	1008	A
2	S2	1017	U
2	S2	1023	A
2	S2	1045	U
2	S2	1049	A
2	S2	1057	C
2	S2	1061	U
2	S2	1062	A
2	S2	1083	A
2	S2	1085	C
2	S2	1089	G
2	S2	1109	C
2	S2	1115	U
2	S2	1116	C
2	S2	1119	A
2	S2	1120	U
2	S2	1123	C
2	S2	1124	C
2	S2	1133	A
2	S2	1138	C
2	S2	1149	A
2	S2	1150	A
2	S2	1153	C
2	S2	1154	U
2	S2	1155	U
2	S2	1168	G

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Mol	Chain	Res	Type
2	S2	1195	A
2	S2	1207	G
2	S2	1208	A
2	S2	1215	C
2	S2	1216	C
2	S2	1217	A
2	S2	1220	A
2	S2	1224	G
2	S2	1237	C
2	S2	1242	U
2	S2	1243	U
2	S2	1251	A
2	S2	1253	A
2	S2	1256	G
2	S2	1257	G
2	S2	1259	A
2	S2	1274	G
2	S2	1275	G
2	S2	1284	A
2	S2	1285	G
2	S2	1286	G
2	S2	1287	A
2	S2	1290	G
2	S2	1293	A
2	S2	1294	G
2	S2	1295	A
2	S2	1298	G
2	S2	1302	G
2	S2	1303	C
2	S2	1305	C
2	S2	1308	U
2	S2	1322	G
2	S2	1332	A
2	S2	1333	U
2	S2	1342	U
2	S2	1348	G
2	S2	1363	C
2	S2	1371	U
2	S2	1372	U
2	S2	1378	A
2	S2	1397	U
2	S2	1415	C

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Mol	Chain	Res	Type
2	S2	1419	C
2	S2	1421	A
2	S2	1422	G
2	S2	1423	C
2	S2	1433	C
2	S2	1435	C
2	S2	1436	C
2	S2	1437	C
2	S2	1438	A
2	S2	1452	A
2	S2	1454	A
2	S2	1463	U
2	S2	1476	A
2	S2	1486	A
2	S2	1489	A
2	S2	1490	G
2	S2	1495	G
2	S2	1497	G
2	S2	1498	A
2	S2	1508	A
2	S2	1510	G
2	S2	1517	G
2	S2	1520	G
2	S2	1521	C
2	S2	1522	A
2	S2	1533	A
2	S2	1537	A
2	S2	1539	U
2	S2	1544	C
2	S2	1552	G
2	S2	1553	C
2	S2	1556	A
2	S2	1570	G
2	S2	1578	U
2	S2	1580	A
2	S2	1587	G
2	S2	1588	A
2	S2	1600	G
2	S2	1601	A
2	S2	1606	G
2	S2	1621	U
2	S2	1623	A

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Mol	Chain	Res	Type
2	S2	1639	G
2	S2	1640	A
2	S2	1648	G
2	S2	1663	A
2	S2	1665	G
2	S2	1679	A
2	S2	1695	A
2	S2	1696	C
2	S2	1719	A
2	S2	1721	U
2	S2	1722	G
2	S2	1724	A
2	S2	1726	G
2	S2	1727	G
2	S2	1729	U
2	S2	1744	G
2	S2	1745	A
2	S2	1749	G
2	S2	1752	C
2	S2	1753	C
2	S2	1754	G
2	S2	1756	C
2	S2	1757	G
2	S2	1758	G
2	S2	1761	U
2	S2	1772	C
2	S2	1773	C
2	S2	1774	C
2	S2	1775	U
2	S2	1777	G
2	S2	1781	A
2	S2	1783	C
2	S2	1784	G
2	S2	1787	G
2	S2	1788	A
2	S2	1789	G
2	S2	1800	A
2	S2	1809	A
2	S2	1810	U
2	S2	1812	U
2	S2	1813	A
2	S2	1822	A

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Mol	Chain	Res	Type
2	S2	1823	A
2	S2	1825	A
2	S2	1826	G
2	S2	1831	A
2	S2	1835	A
2	S2	1838	U
2	S2	1849	G
2	S2	1850	A
2	S2	1852	C
2	S2	1861	G
2	S2	1862	G
2	S2	1863	A
2	S2	1864	U
2	S2	1865	C
2	S2	1867	U
2	S2	1869	A

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	S2	112	U
2	S2	291	G
2	S2	688	U
2	S2	1434	C

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 25 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

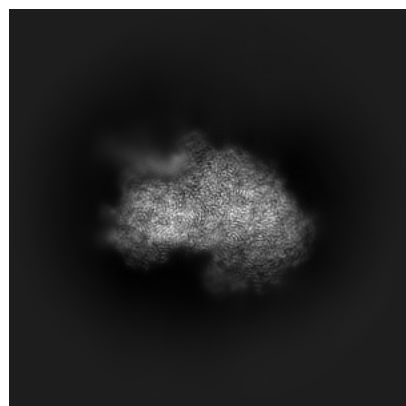
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38752. These allow visual inspection of the internal detail of the map and identification of artifacts.

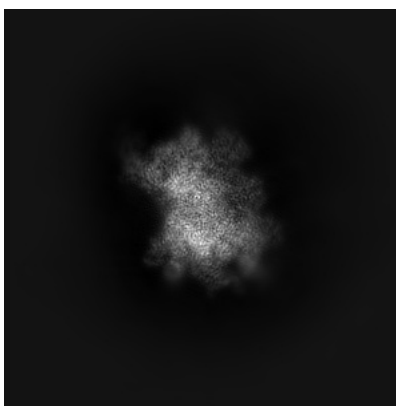
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

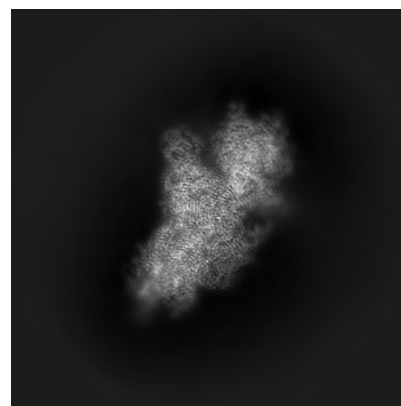
6.1.1 Primary map



X

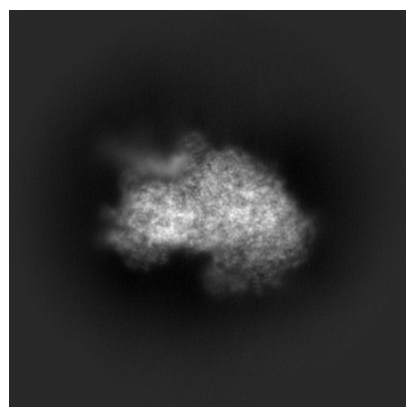


Y

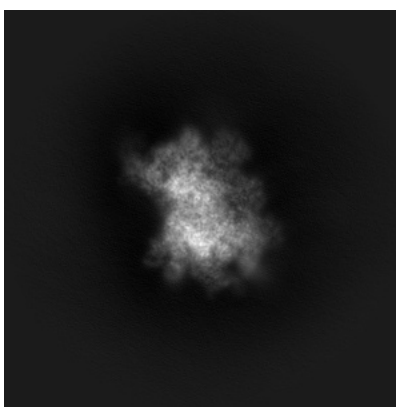


Z

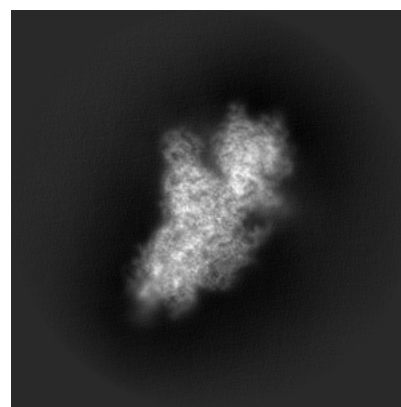
6.1.2 Raw map



X



Y

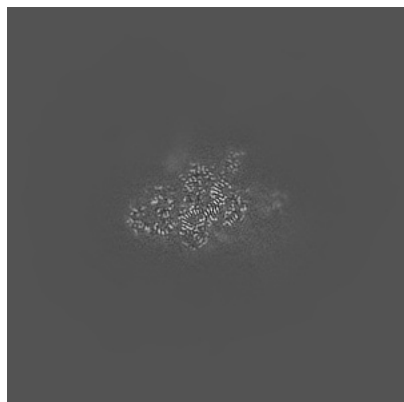


Z

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

6.2 Central slices [i](#)

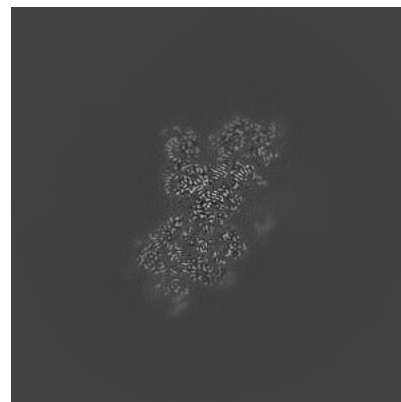
6.2.1 Primary map



X Index: 210

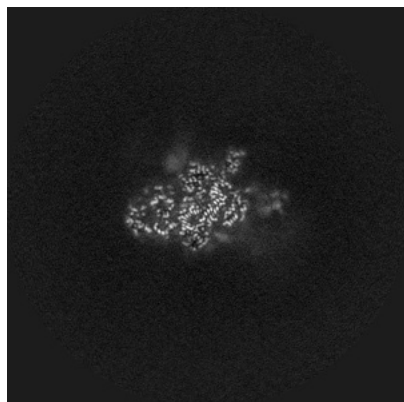


Y Index: 210

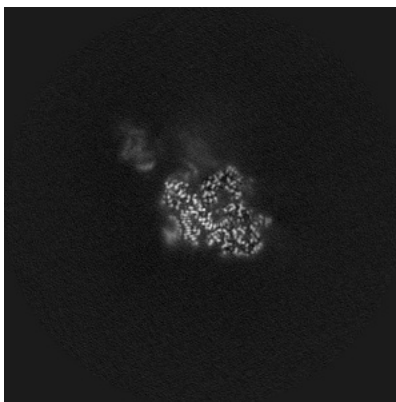


Z Index: 210

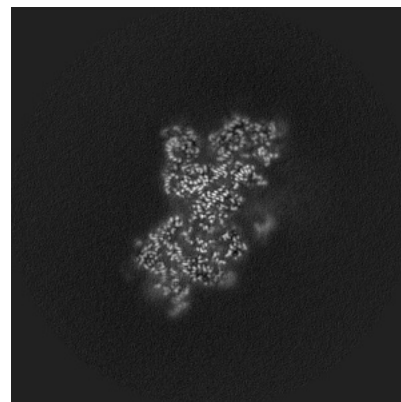
6.2.2 Raw map



X Index: 210



Y Index: 210

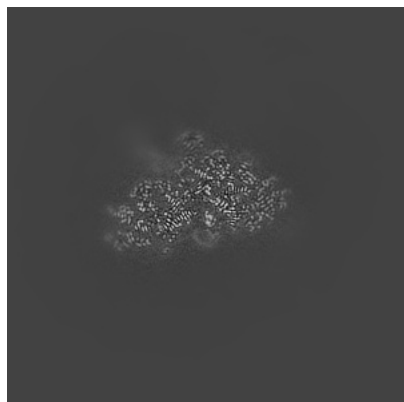


Z Index: 210

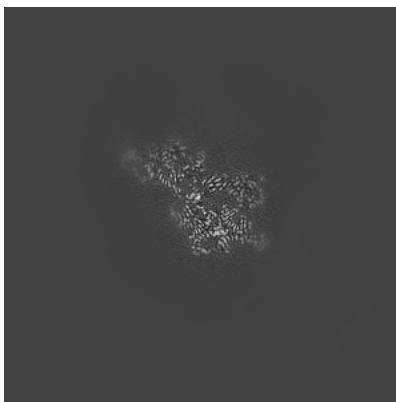
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

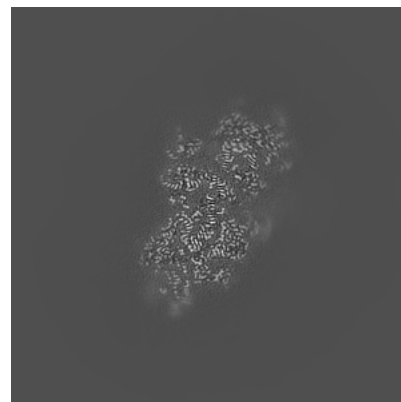
6.3.1 Primary map



X Index: 185

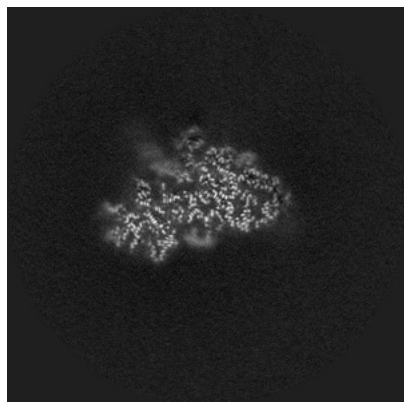


Y Index: 233

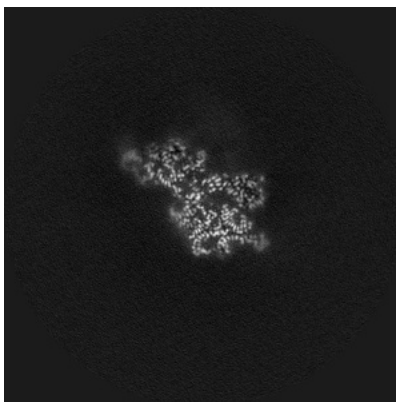


Z Index: 204

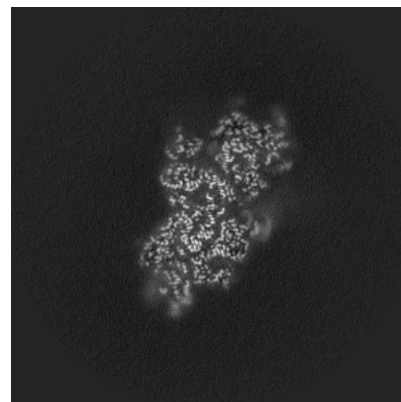
6.3.2 Raw map



X Index: 179



Y Index: 233

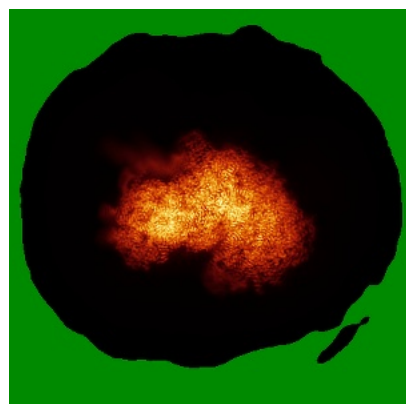


Z Index: 204

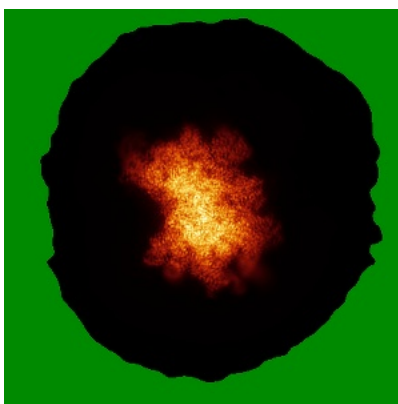
The images above show the largest variance slices of the map in three orthogonal directions.

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

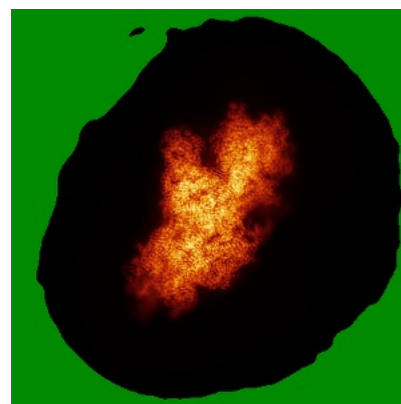
6.4.1 Primary map



X



Y

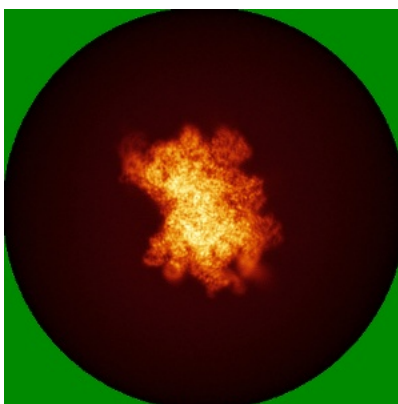


Z

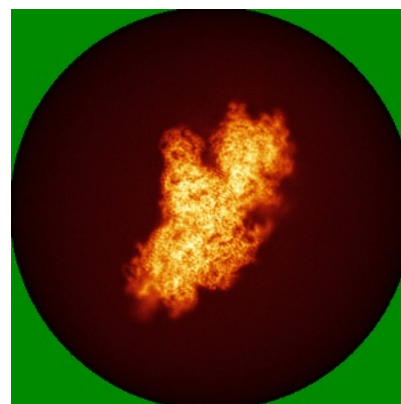
6.4.2 Raw map



X



Y

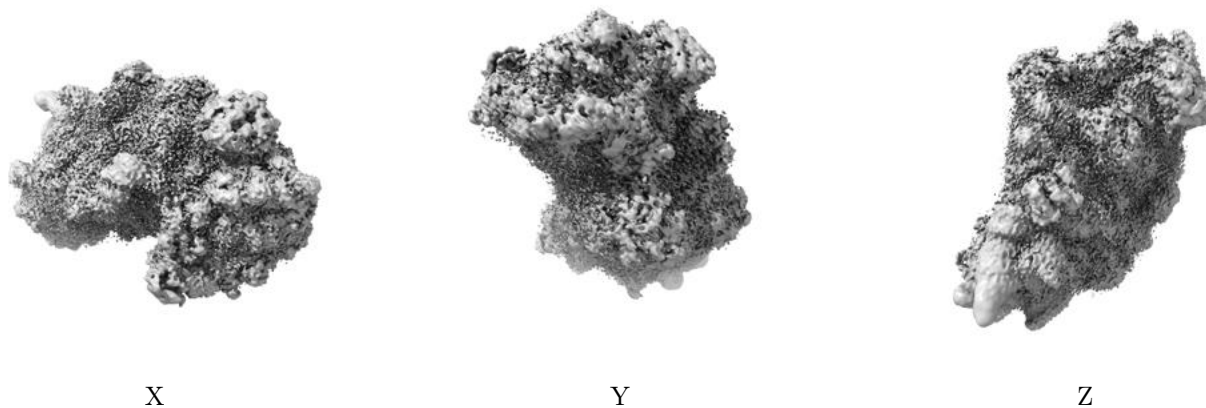


Z

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

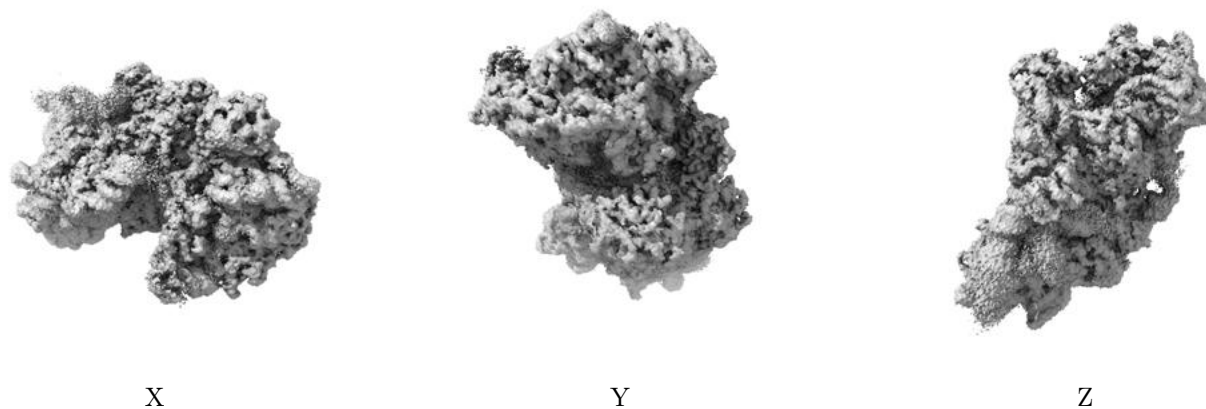
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

6.5.2 Raw map



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

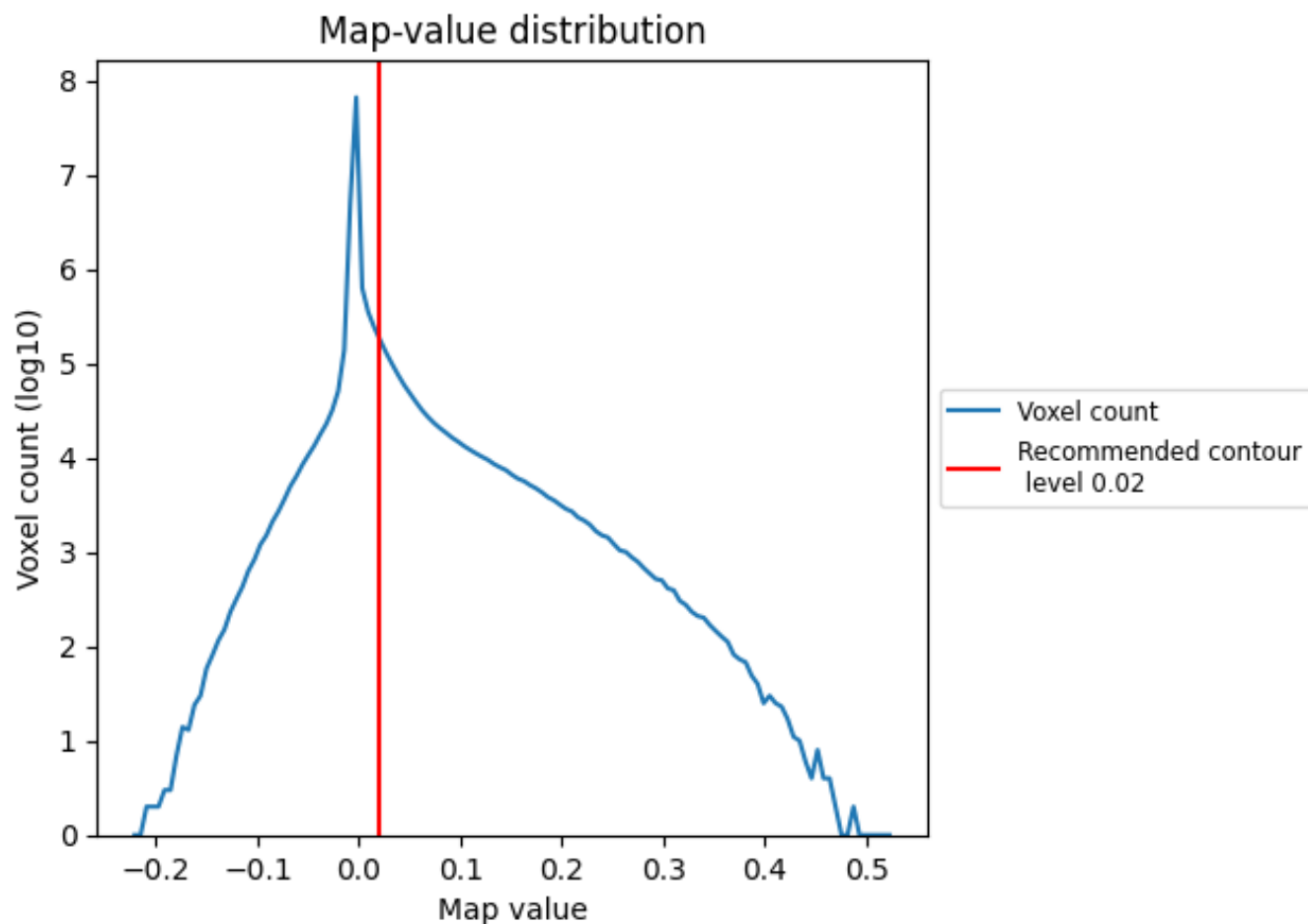
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

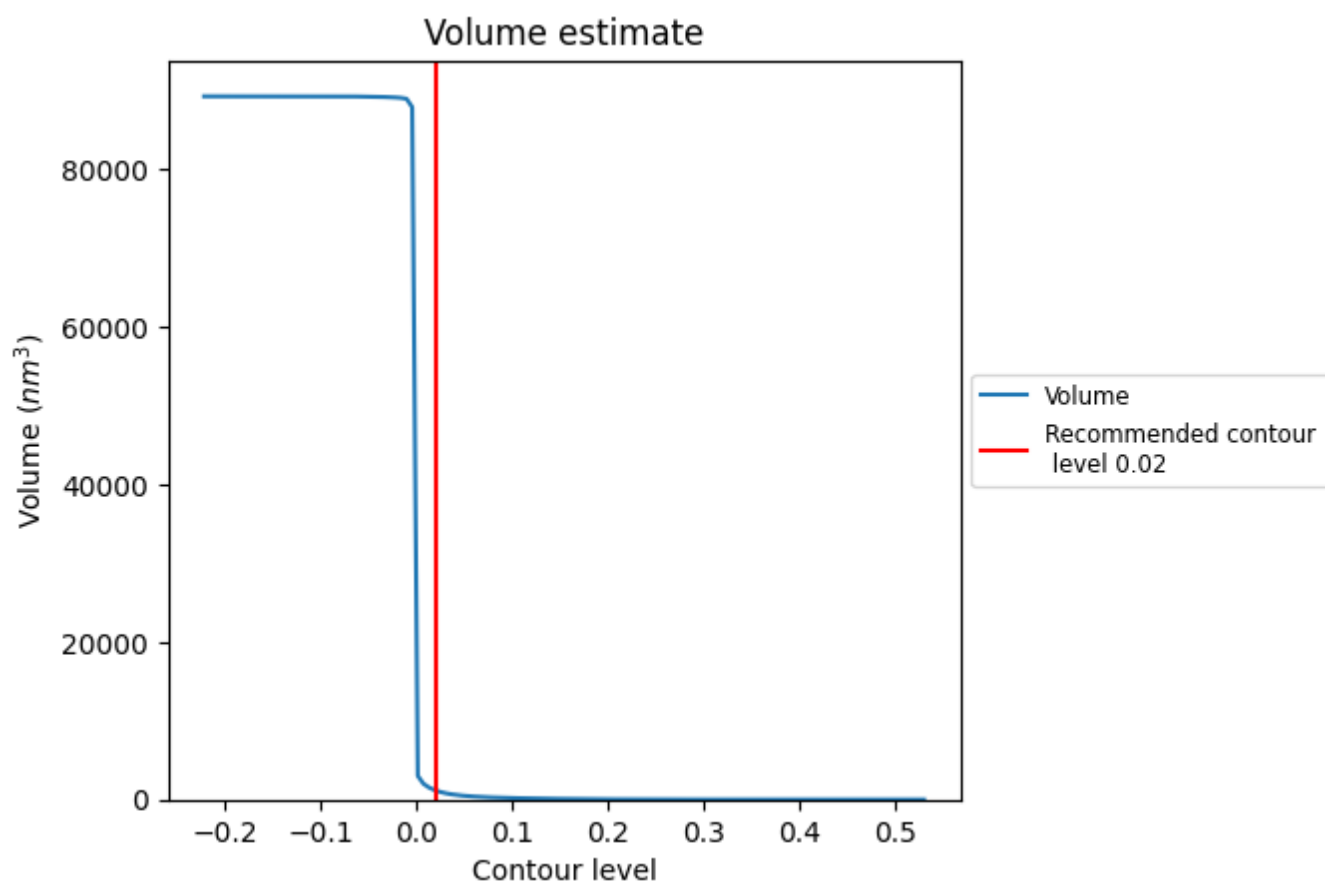
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

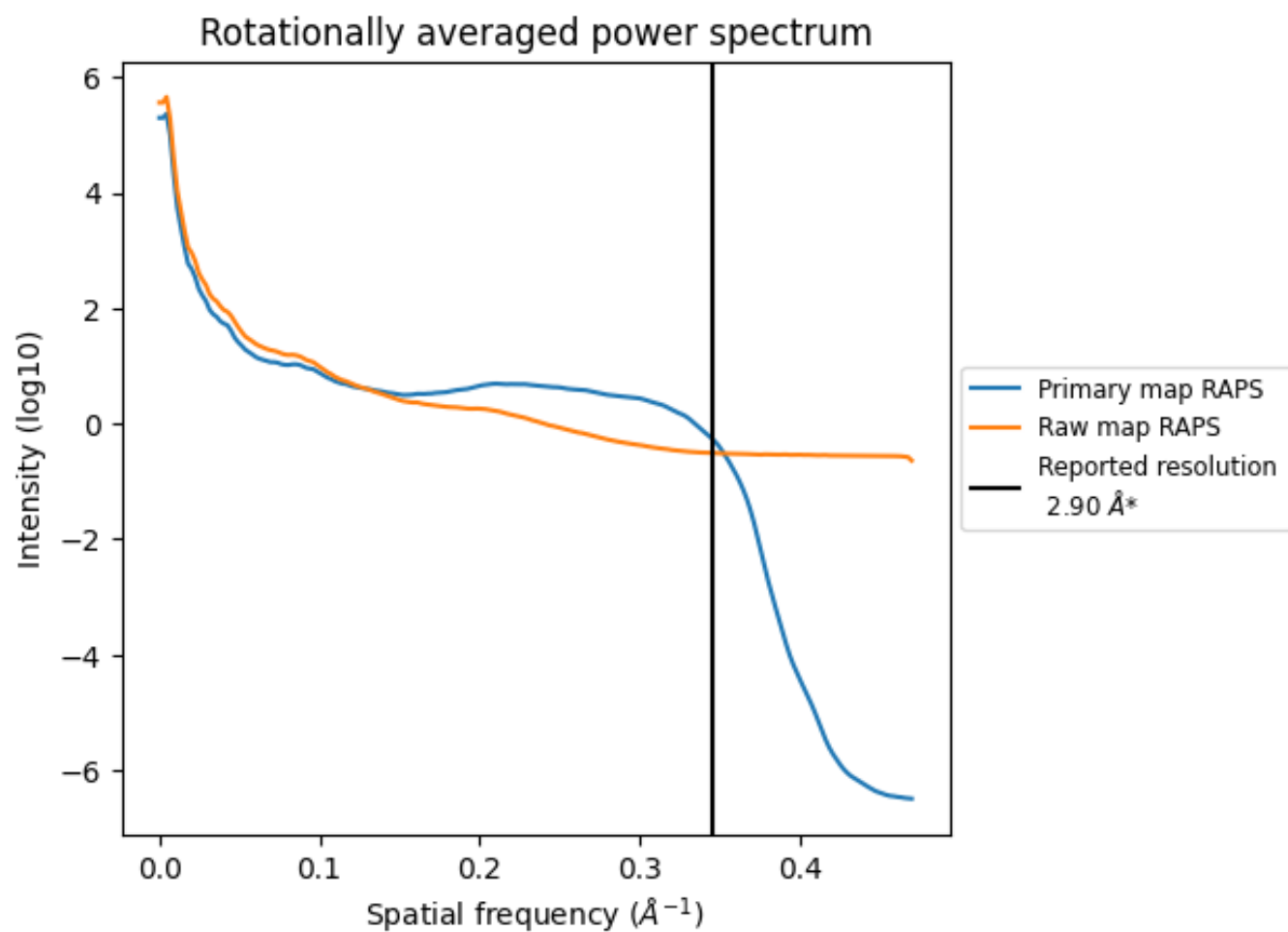
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1172 nm^3 ; this corresponds to an approximate mass of 1059 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 ⓘ

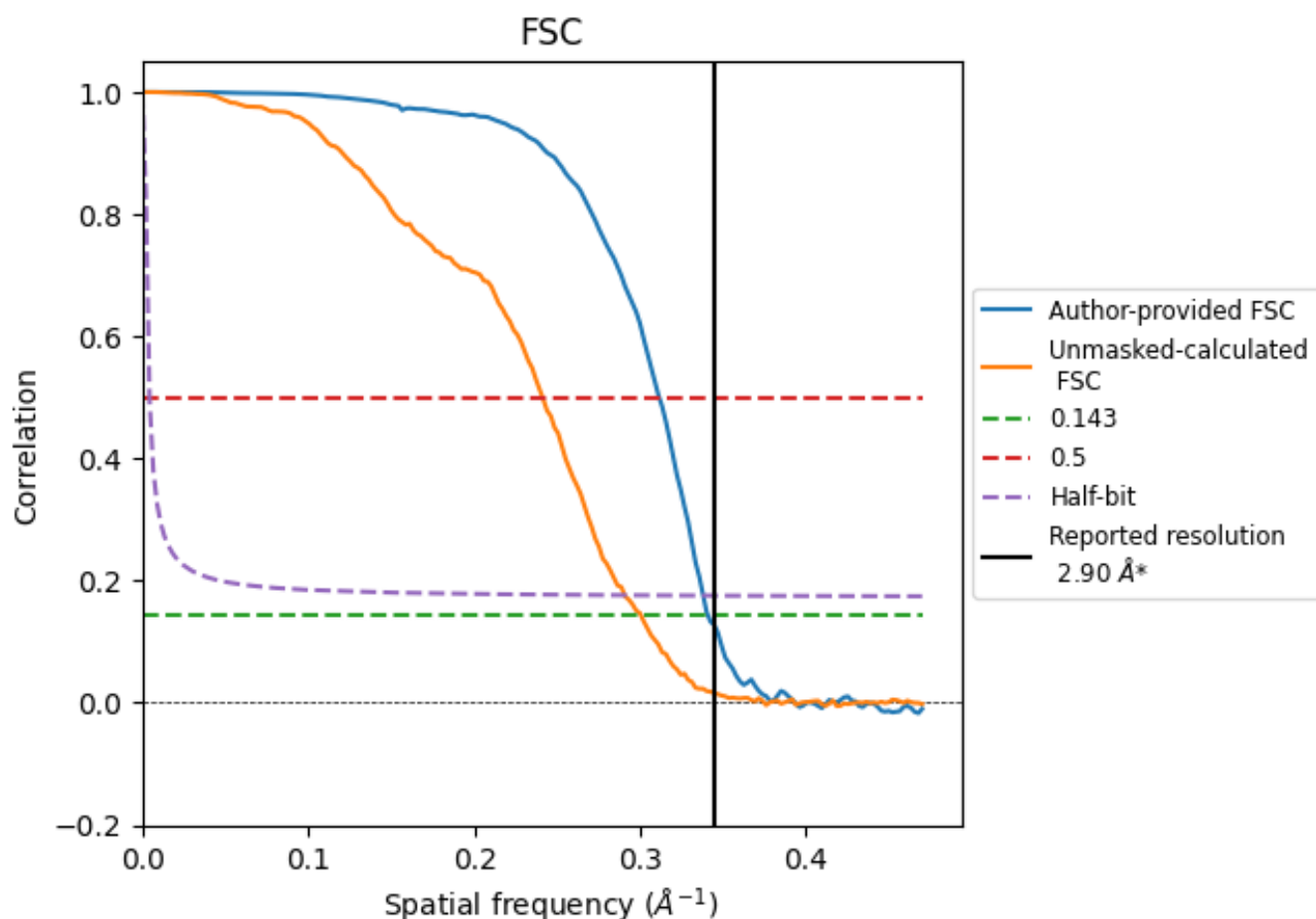


*Reported resolution corresponds to spatial frequency of $0.345 \text{ \AA}^{-1}$

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 0.345 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

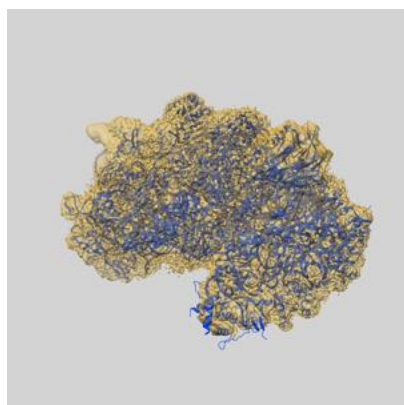
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.93	3.21	2.96
Unmasked-calculated*	3.33	4.15	3.44

*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 3.33 differs from the reported value 2.9 by more than 10 %

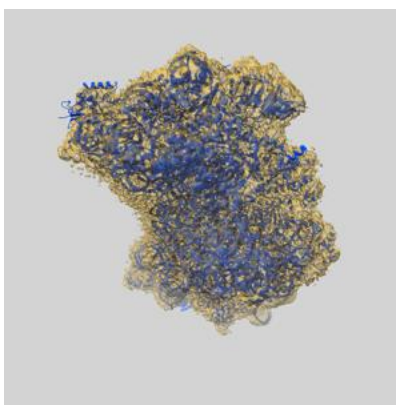
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38752 and PDB model 8XXL. Per-residue inclusion information can be found in section 3 on page 11.

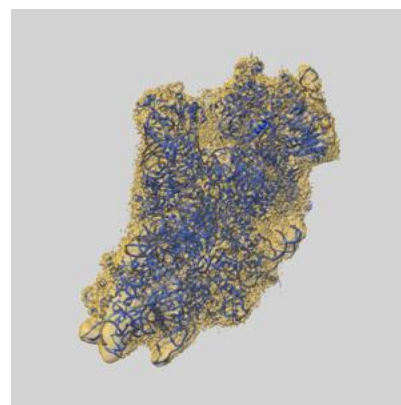
9.1 Map-model overlay [i](#)



X



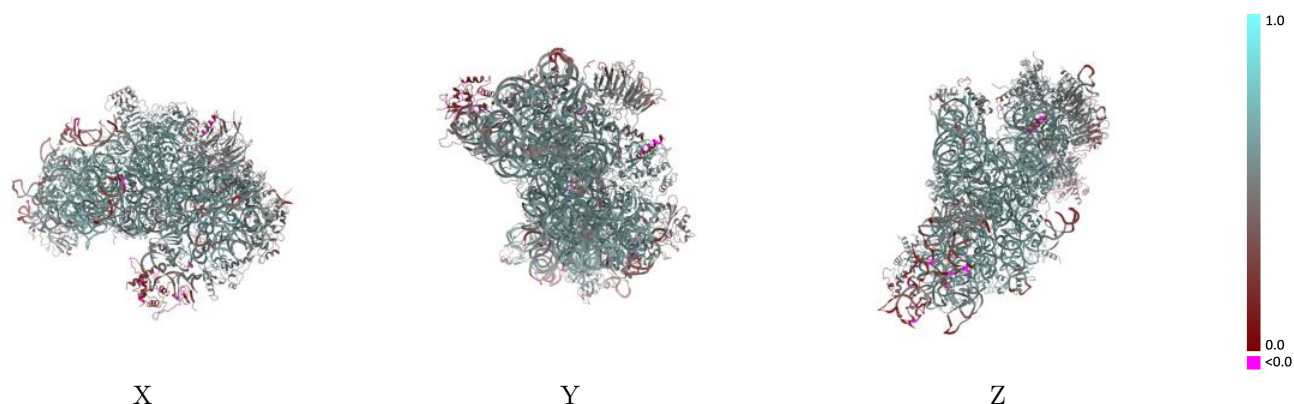
Y



Z

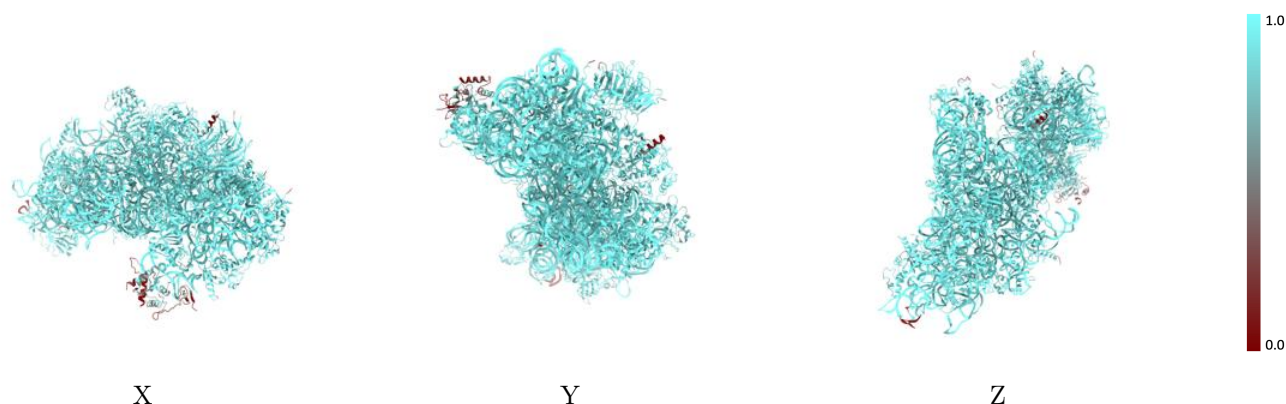
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



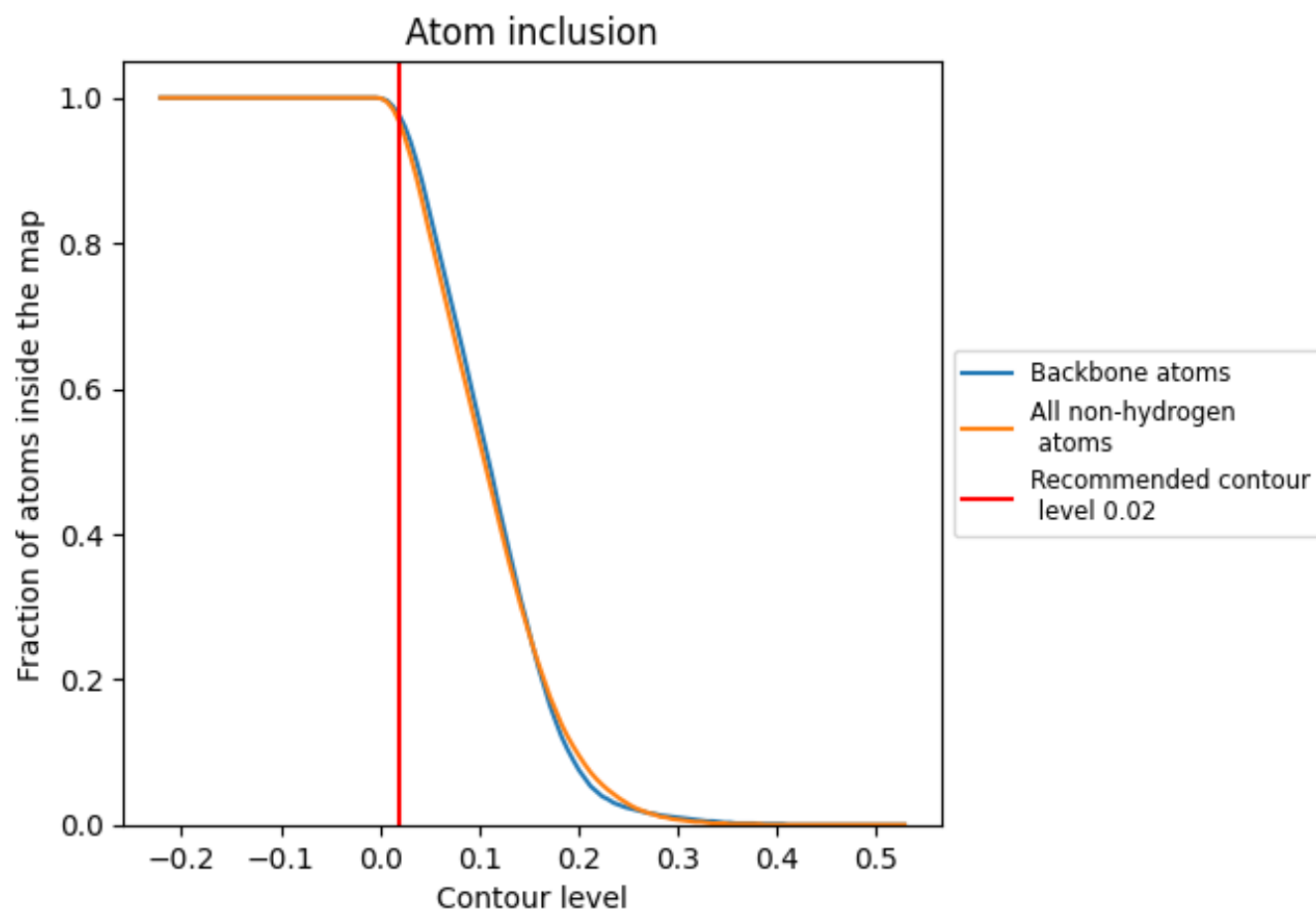
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion ⓘ



At the recommended contour level, 98% of all backbone atoms, 97% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9660	 0.5380
CD	 0.9700	 0.5470
Ln	 0.9330	 0.5230
S2	 0.9900	 0.5570
SA	 0.9430	 0.5540
SB	 0.9670	 0.5380
SC	 0.9820	 0.5950
SD	 0.9700	 0.5480
SE	 0.9930	 0.6000
SF	 0.9550	 0.5010
SG	 0.9730	 0.4920
SH	 0.9090	 0.4610
SI	 0.9690	 0.5250
SJ	 0.9790	 0.5950
SK	 0.9630	 0.5090
SL	 0.9630	 0.5660
SM	 0.5000	 0.1850
SN	 0.9940	 0.5810
SO	 0.9410	 0.5330
SP	 0.9610	 0.5180
SQ	 0.9750	 0.5670
SR	 0.9450	 0.5130
SS	 0.9450	 0.4940
ST	 0.9670	 0.5290
SU	 0.9530	 0.4950
SV	 0.9840	 0.5570
SW	 0.9920	 0.6190
SX	 0.9900	 0.6080
SY	 0.9620	 0.5490
SZ	 0.9310	 0.4650
Sa	 0.9720	 0.5660
Sb	 0.9550	 0.4990
Sc	 0.9360	 0.4540
Sd	 0.9680	 0.5510
Se	 0.9530	 0.5320



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Chain	Atom inclusion	Q-score
Sf	 0.3150	 0.1340
Sg	 0.9510	 0.4360