Full wwPDB EM Validation Report ⓘ

Apr 22, 2024 – 02:39 PM JST

PDB ID	:	8XXL
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:

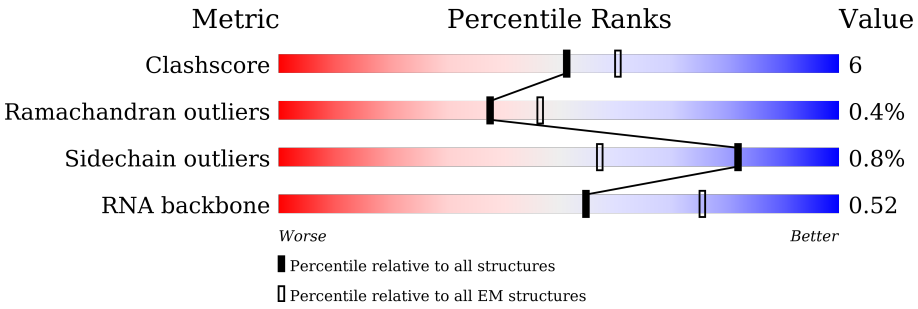
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.90 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 <=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	96%
2	S2	1869	56% 30% 5% 8%
3	SA	295	62% 13% 25%
4	SB	264	68% 13% 19%
5	SD	243	76% 17% 7%
6	SE	263	82% 17%
7	SF	204	81% 11% 7%

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Mol	Chain	Length	Quality of chain
8	SH	194	70% 23%
9	SI	208	87% 12%
10	SK	165	52% 7% 41%
11	SL	158	78% 18%
12	SP	145	76% 8% 17%
13	SQ	146	79% 18%
14	SR	135	92% 8%
15	SS	152	72% 24% 5%
16	ST	145	79% 20%
17	SU	119	75% 13% 13%
18	SV	83	84% 16%
19	SX	143	84% 14%
20	Sa	115	88% 11%
21	Sc	69	90% 7%
22	Sd	56	93% 5%
23	Sg	317	99%
24	SC	293	64% 12% 24%
25	SG	249	78% 17% 5%
26	SJ	194	87% 8% 5%
27	SM	132	33% 76% 17% 8%
28	SN	151	89% 11%
29	SO	151	77% 16% 7%
30	SW	130	92% 8%
31	SY	133	81% 17%
32	SZ	125	44% 12% 40%

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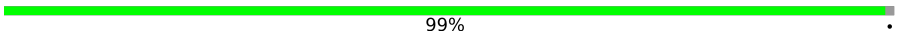
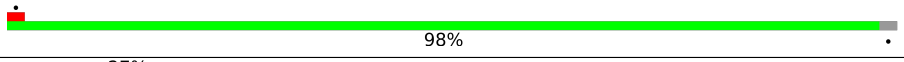
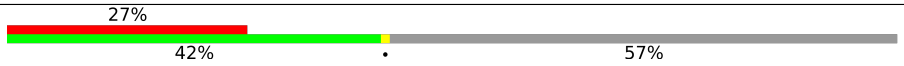
Mol	Chain	Length	Quality of chain
33	Sb	84	
34	Se	59	
35	Sf	156	
36	CD	469	

2 Entry composition (i)

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 (three-letter code: 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 (three-letter code: ZN) (formula: Zn).

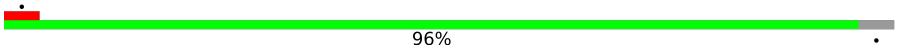
Mol	Chain	Residues	Atoms		AltConf
38	Sa	1	Total	Zn	0
			1	1	
38	Sd	1	Total	Zn	0
			1	1	
38	Sf	1	Total	Zn	0
			1	1	

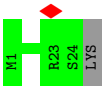
3 Residue-property plots (i)

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

- Molecule 1: 60S ribosomal protein L41

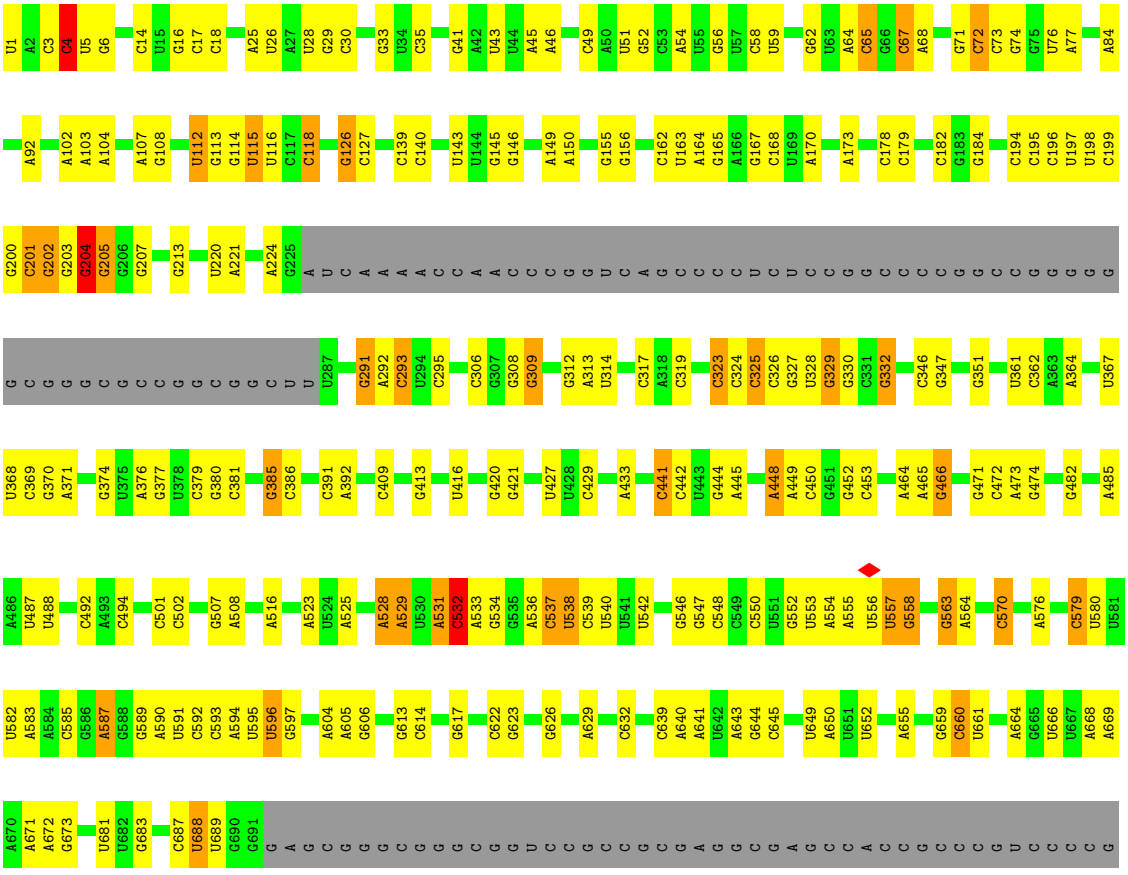
Chain Ln:

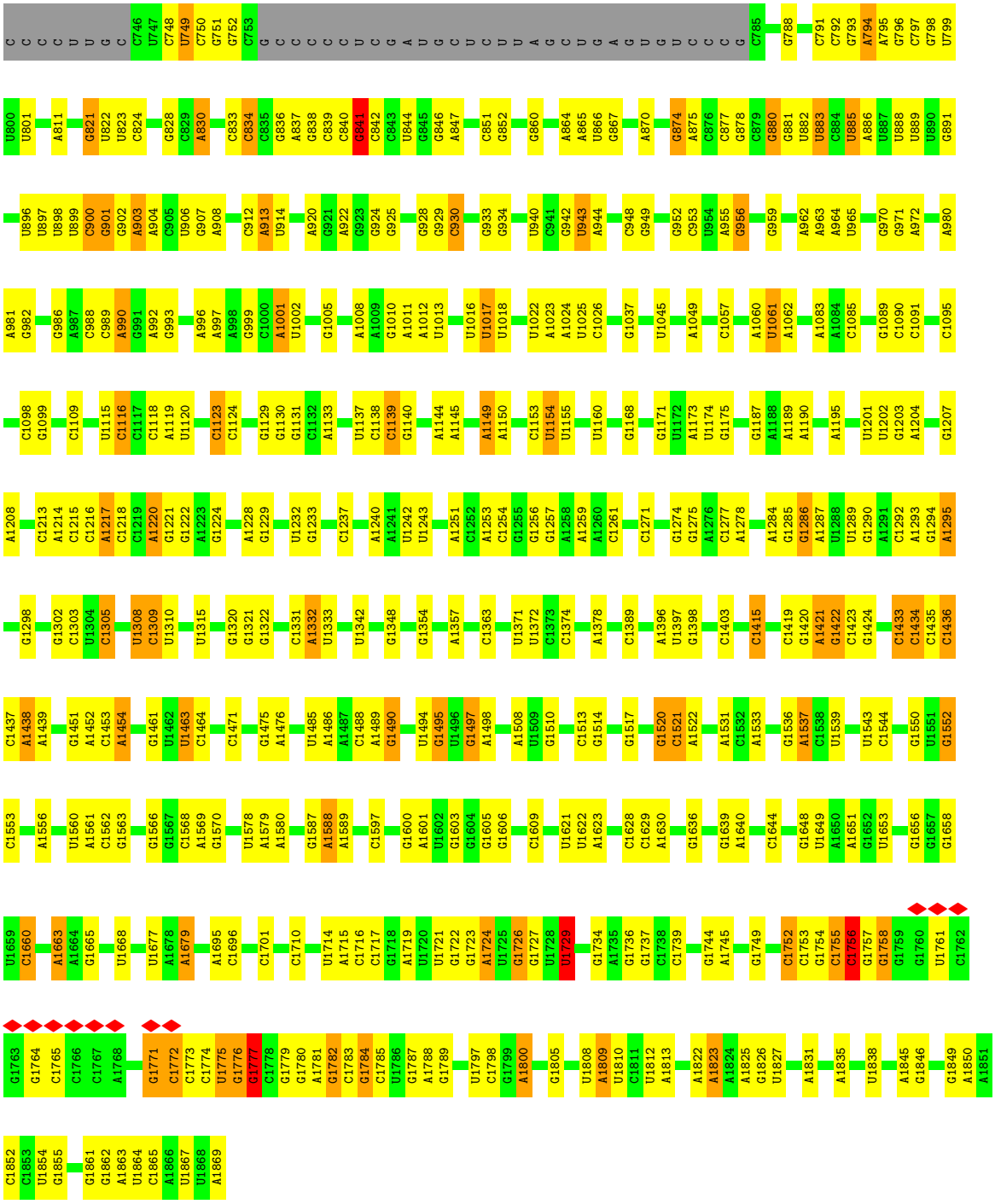




- Molecule 2: 18S rRNA

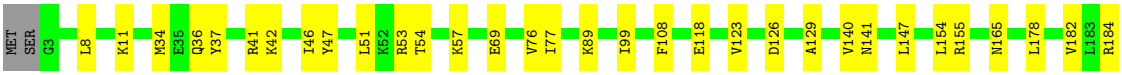
Chain S2:

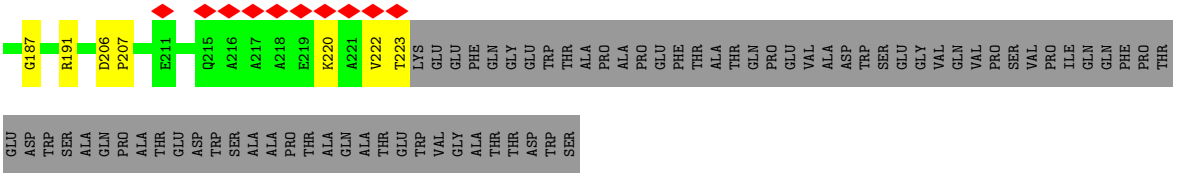




• Molecule 3: 40S ribosomal protein SA

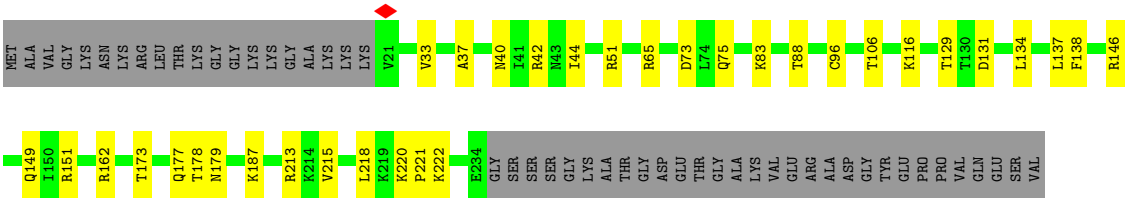
Chain SA:





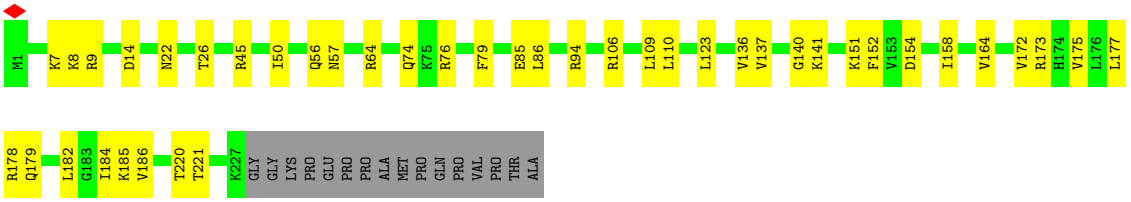
• Molecule 4: 40S ribosomal protein S3a

Chain SB:



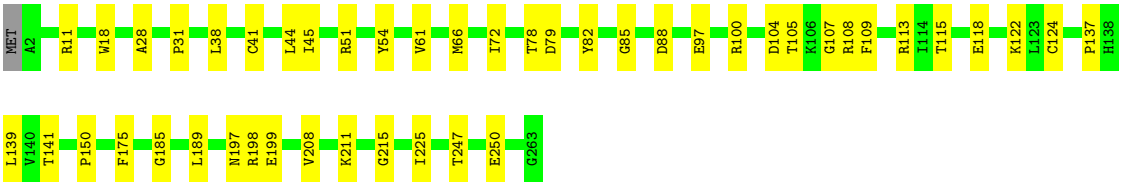
• Molecule 5: 40S ribosomal protein S3

Chain SD:



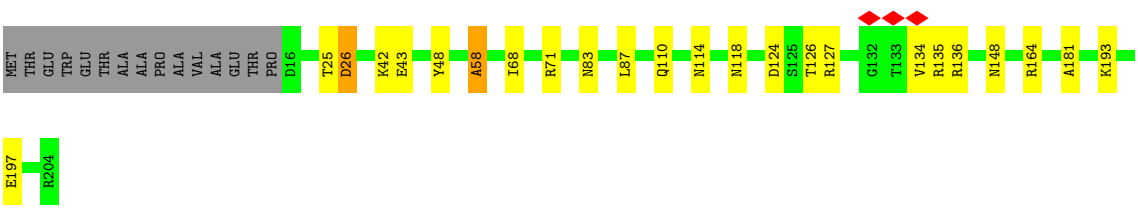
• Molecule 6: 40S ribosomal protein S4, X isoform

Chain SE:



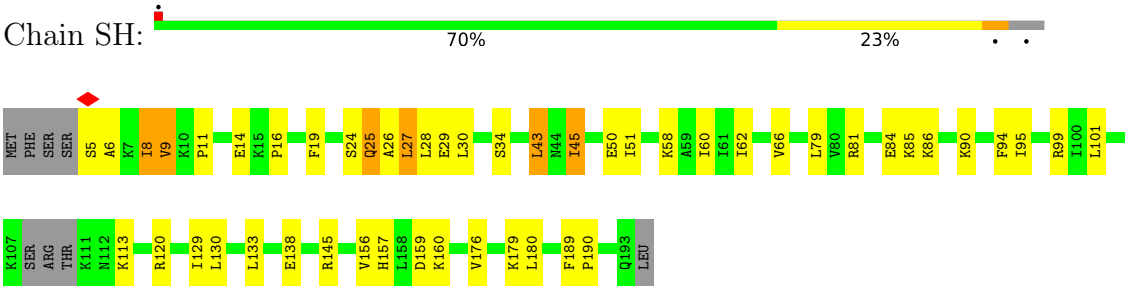
• Molecule 7: 40S ribosomal protein S5

Chain SF:



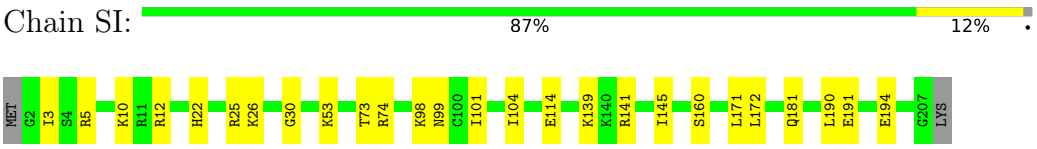
• Molecule 8: 40S ribosomal protein S7

Chain SH:



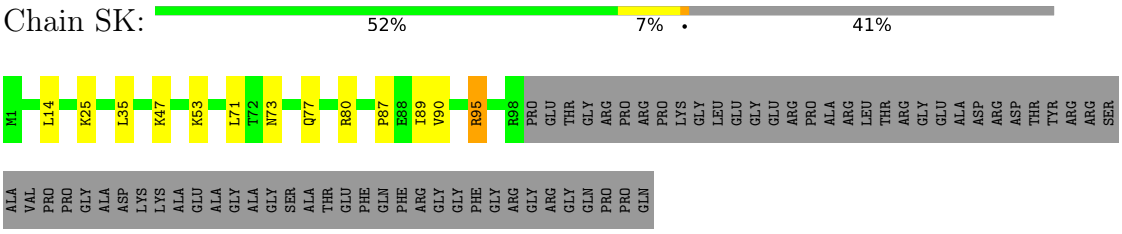
• Molecule 9: 40S ribosomal protein S8

Chain SI:



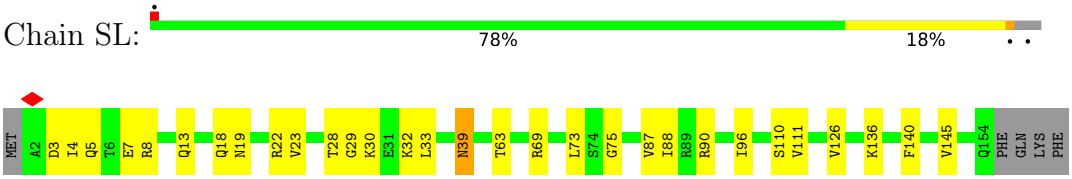
• Molecule 10: 40S ribosomal protein S10

Chain SK:



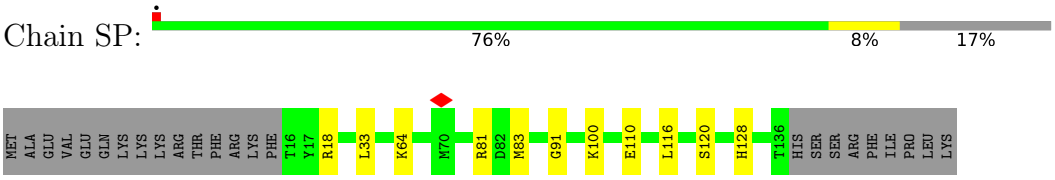
• Molecule 11: 40S ribosomal protein S11

Chain SL:



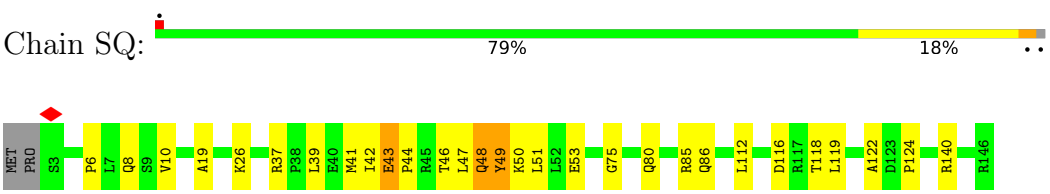
• Molecule 12: 40S ribosomal protein S15

Chain SP:



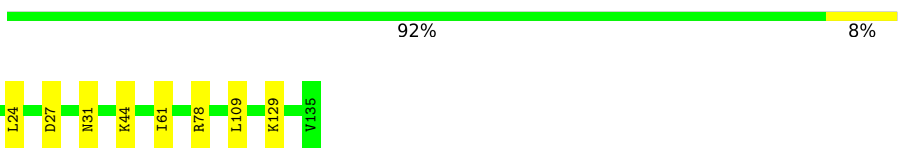
• Molecule 13: 40S ribosomal protein S16

Chain SQ:



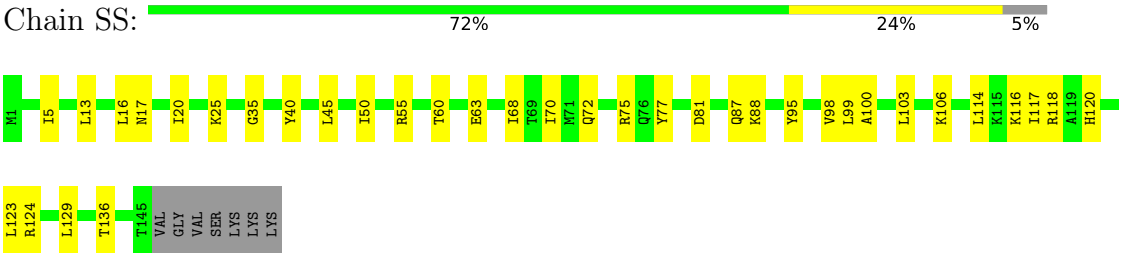
• Molecule 14: 40S ribosomal protein S17

Chain SR:



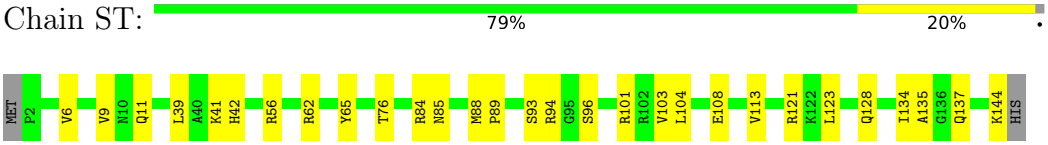
• Molecule 15: 40S ribosomal protein S18

Chain SS:



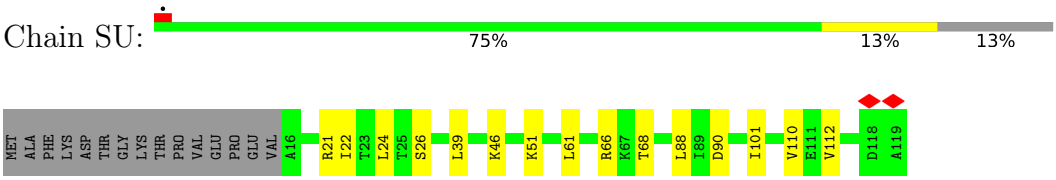
• Molecule 16: 40S ribosomal protein S19

Chain ST:



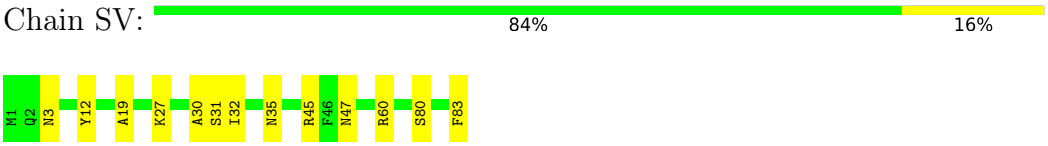
• Molecule 17: 40S ribosomal protein S20

Chain SU:



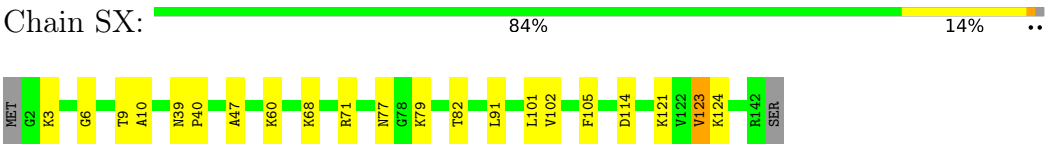
• Molecule 18: 40S ribosomal protein S21

Chain SV:



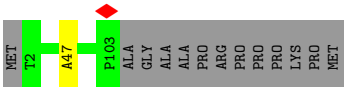
• Molecule 19: 40S ribosomal protein S23

Chain SX:



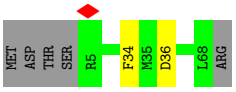
• Molecule 20: 40S ribosomal protein S26

Chain Sa:



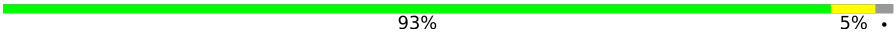
• Molecule 21: 40S ribosomal protein S28

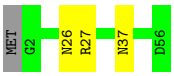
Chain Sc:



• Molecule 22: 40S ribosomal protein S29

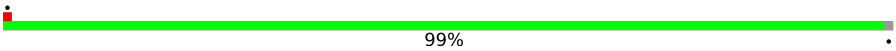
Chain Sd:

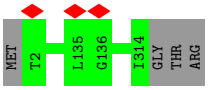




• Molecule 23: Receptor of activated protein C kinase 1

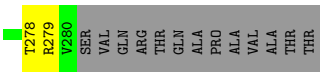
Chain Sg:





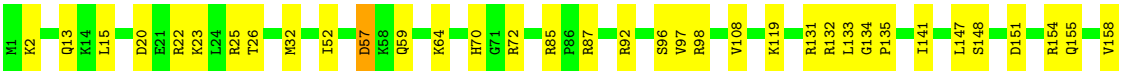
• Molecule 24: 40S ribosomal protein S2

Chain SC:



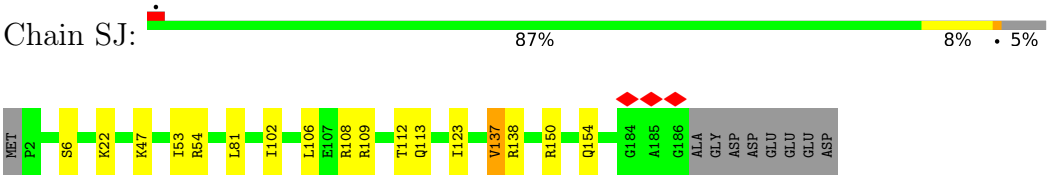
• Molecule 25: 40S ribosomal protein S6

Chain SG:



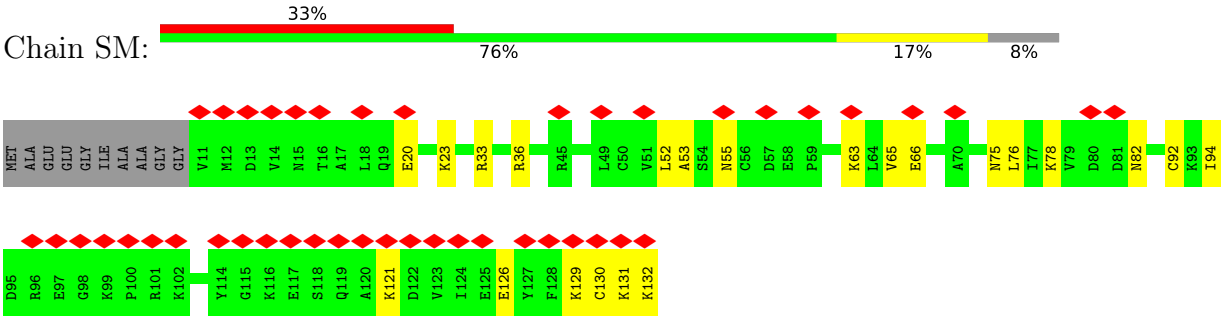
• Molecule 26: 40S ribosomal protein S9

Chain SJ:



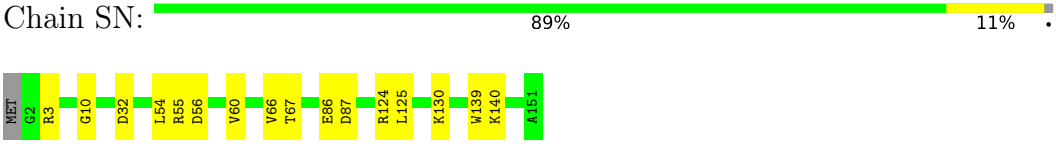
• Molecule 27: 40S ribosomal protein S12

Chain SM:



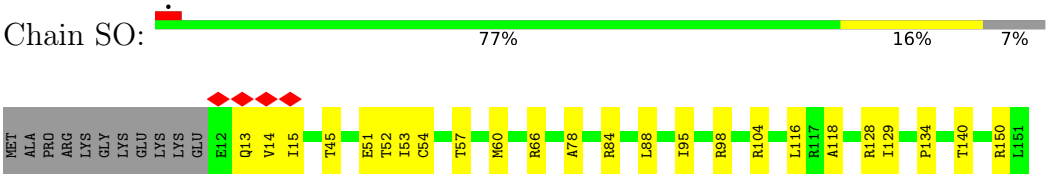
• Molecule 28: 40S ribosomal protein S13

Chain SN:



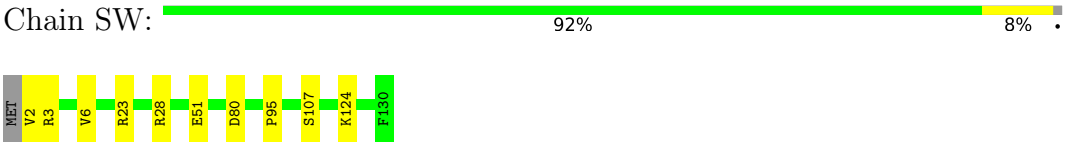
• Molecule 29: 40S ribosomal protein S14

Chain SO:



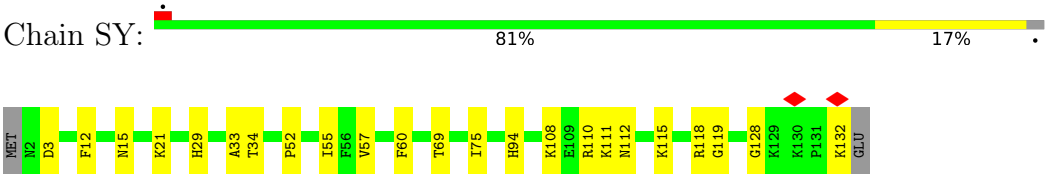
• Molecule 30: 40S ribosomal protein S15a

Chain SW:



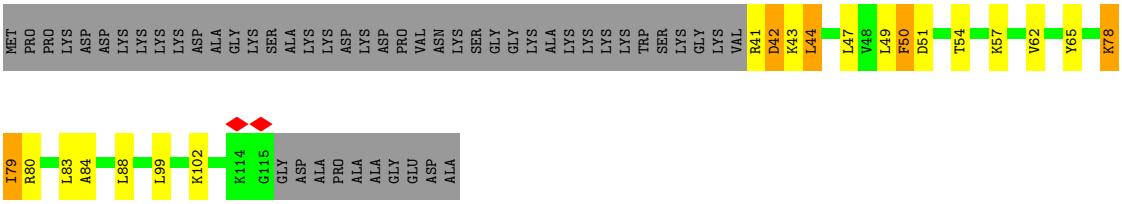
• Molecule 31: 40S ribosomal protein S24

Chain SY:



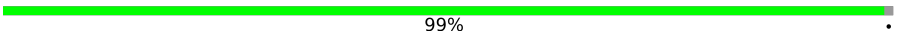
• Molecule 32: 40S ribosomal protein S25

Chain SZ:



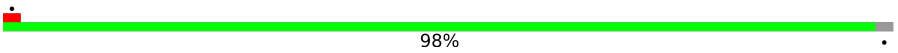
• Molecule 33: 40S ribosomal protein S27

Chain Sb:



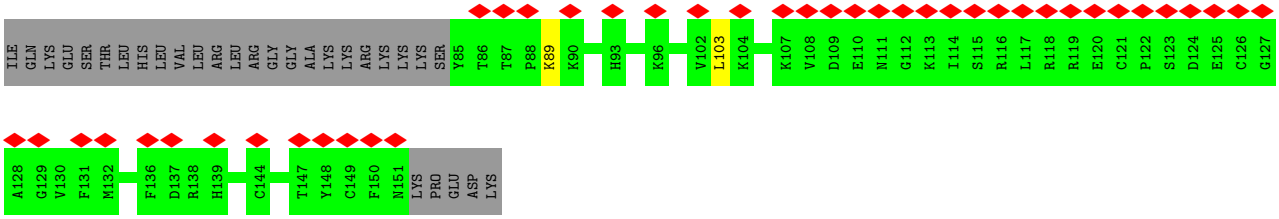
• Molecule 34: 40S ribosomal protein S30

Chain Se:



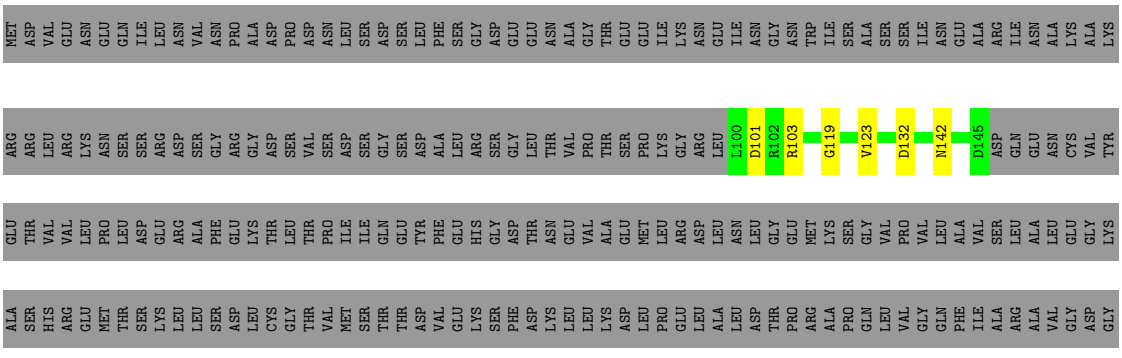
• Molecule 35: Ubiquitin-40S ribosomal protein S27a

Chain Sf:



• Molecule 36: Programmed cell death protein 4

Chain CD:



ILE LEU CYS ASN THR TYR ILE ASP SER TYR LYS GLY THR VAL ASP CYS VAL GLN ALA ARG ALA ALA LEU ASP LYS ALA THR VAL LEU LEU SER MET SER LYS GLY GLY LYS ARG LYS ASP SER VAL TRP GLY SER GLY GLY GLN GLN SER VAL ASN HIS LEU VAL LYS GLU ILE ASP

MET LEU LEU LYS GLU TYR LEU LEU SER GLY ASP ILE SER GLU ALA GLU HIS CYS LEU LYS GLU LEU GLU VAL PRO HIS PHE HIS HIS GLU LEU VAL TYR GLU ALA ILE ILE MET VAL LEU GLU SER THR GLY GLU SER THR PHE LYS MET ILE LEU ASP LEU LEU LYS SER LEU TRP LYS

SER SER THR ILE THR VAL ASP GLN MET LYS ARG GLY TYR GLU ARG ILE TYR ASN GLU ILE PRO ASP ILE ASN LEU ASP VAL PRO HIS SER TYR SER VAL LEU GLU ARG PHE VAL GLU GLU CYS PHE GLN ALA GLY ILE ILE SER LYS GLN LEU ARG ASP LEU CYS PRO SER ARG GLY ARG

LYS ARG PHE VAL SER GLU GLY ASP GLY GLY ARG LEU LYS PRO GLU SER TYR

4 Experimental information (i)

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 ($e^-/Å^2$)	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 (Å)	446.88, 446.88, 446.88	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.064, 1.064, 1.064	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.25	0/231	0.78	0/294
2	S2	0.43	0/40843	0.99	133/63639 (0.2%)
3	SA	0.33	0/1778	0.58	1/2416 (0.0%)
4	SB	0.29	0/1765	0.59	0/2362
5	SD	0.30	0/1793	0.61	2/2414 (0.1%)
6	SE	0.31	0/2118	0.60	1/2849 (0.0%)
7	SF	0.28	0/1516	0.62	1/2037 (0.0%)
8	SH	0.37	0/1519	0.60	0/2033
9	SI	0.29	0/1715	0.62	0/2287
10	SK	0.28	0/851	0.56	0/1147
11	SL	0.31	0/1268	0.59	0/1696
12	SP	0.28	0/1003	0.60	0/1342
13	SQ	0.36	0/1160	0.67	0/1553
14	SR	0.30	0/1105	0.63	1/1484 (0.1%)
15	SS	0.32	0/1216	0.66	0/1628
16	ST	0.28	0/1131	0.56	0/1515
17	SU	0.27	0/831	0.64	0/1115
18	SV	0.31	0/643	0.63	0/860
19	SX	0.37	0/1116	0.61	0/1490
20	Sa	0.32	0/836	0.66	0/1121
21	Sc	0.37	0/508	0.70	0/680
22	Sd	0.43	0/470	0.72	0/623
23	Sg	0.26	0/2493	0.61	0/3394
24	SC	0.33	0/1762	0.59	0/2381
25	SG	0.28	0/1946	0.64	1/2590 (0.0%)
26	SJ	0.29	0/1550	0.60	0/2069
27	SM	0.25	0/950	0.55	0/1275
28	SN	0.29	0/1232	0.57	1/1656 (0.1%)
29	SO	0.30	0/1062	0.63	0/1425
30	SW	0.30	0/1051	0.59	0/1406
31	SY	0.31	0/1083	0.60	0/1438
32	SZ	0.45	0/604	0.74	0/810

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
33	Sb	0.27	0/665	0.57	0/891
34	Se	0.27	0/465	0.59	0/612
35	Sf	0.27	0/560	0.66	1/745 (0.1%)
36	CD	0.27	0/352	0.63	0/471
All	All	0.37	0/81191	0.84	142/117748 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
22	Sd	0	1
26	SJ	0	1
31	SY	0	1
All	All	0	3

There are no bond length outliers.

All (142) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	S2	1772	C	N3-C2-O2	-13.03	112.78	121.90
2	S2	1772	C	N1-C2-O2	12.86	126.61	118.90
2	S2	1782	G	N1-C6-O6	-12.43	112.44	119.90
2	S2	501	C	N1-C2-O2	11.81	125.98	118.90
2	S2	293	C	N1-C2-O2	11.55	125.83	118.90
2	S2	501	C	C2-N1-C1'	11.19	131.11	118.80
2	S2	1782	G	C5-C6-O6	11.09	135.25	128.60
2	S2	195	C	N3-C2-O2	-11.01	114.19	121.90
2	S2	293	C	C2-N1-C1'	10.22	130.04	118.80
2	S2	1453	C	C2-N1-C1'	9.99	129.79	118.80
2	S2	1453	C	N1-C2-O2	9.87	124.82	118.90
2	S2	537	C	C2-N1-C1'	9.87	129.65	118.80
2	S2	882	U	N1-C2-O2	9.72	129.61	122.80
2	S2	501	C	N3-C2-O2	-9.40	115.32	121.90
2	S2	882	U	N3-C2-O2	-9.19	115.77	122.20
2	S2	883	U	N3-C2-O2	-9.16	115.79	122.20
2	S2	293	C	N3-C2-O2	-8.27	116.11	121.90
2	S2	1772	C	C6-N1-C2	-8.25	117.00	120.30
2	S2	118	C	C2-N1-C1'	8.13	127.74	118.80
2	S2	118	C	N1-C2-O2	8.07	123.74	118.90
2	S2	195	C	N1-C2-O2	7.96	123.68	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	S2	1756	C	N3-C2-O2	-7.89	116.38	121.90
2	S2	1139	C	N3-C2-O2	-7.82	116.42	121.90
2	S2	501	C	C6-N1-C1'	-7.71	111.54	120.80
2	S2	834	C	N3-C2-O2	-7.68	116.52	121.90
2	S2	882	U	C2-N1-C1'	7.59	126.81	117.70
2	S2	1139	C	N1-C2-O2	7.48	123.39	118.90
2	S2	537	C	C6-N1-C1'	-7.43	111.88	120.80
2	S2	1453	C	N3-C2-O2	-7.42	116.70	121.90
2	S2	501	C	C6-N1-C2	-7.42	117.33	120.30
2	S2	293	C	C6-N1-C1'	-7.35	111.98	120.80
2	S2	537	C	N1-C2-O2	7.16	123.20	118.90
2	S2	1139	C	C2-N1-C1'	7.09	126.60	118.80
2	S2	1520	G	C4-N9-C1'	7.08	135.70	126.50
2	S2	1453	C	C6-N1-C1'	-7.05	112.34	120.80
2	S2	688	U	P-O3'-C3'	7.05	128.16	119.70
2	S2	1756	C	C5-C4-N4	7.02	125.11	120.20
2	S2	883	U	C2-N1-C1'	6.92	126.01	117.70
2	S2	883	U	N1-C2-O2	6.90	127.63	122.80
14	SR	109	LEU	CA-CB-CG	6.78	130.89	115.30
2	S2	1139	C	C6-N1-C2	-6.76	117.60	120.30
2	S2	1016	U	C2-N1-C1'	6.72	125.76	117.70
2	S2	1755	C	C2-N1-C1'	6.66	126.13	118.80
2	S2	118	C	N3-C2-O2	-6.65	117.24	121.90
2	S2	1772	C	C2-N1-C1'	6.64	126.11	118.80
2	S2	1389	C	C2-N1-C1'	6.62	126.08	118.80
2	S2	1756	C	N3-C4-N4	-6.60	113.38	118.00
2	S2	1271	C	N1-C2-O2	6.57	122.84	118.90
2	S2	1016	U	N1-C2-O2	6.57	127.40	122.80
2	S2	1755	C	N1-C2-O2	6.51	122.81	118.90
2	S2	427	U	C2-N1-C1'	6.50	125.50	117.70
2	S2	1756	C	C6-N1-C2	-6.50	117.70	120.30
2	S2	1332	A	O5'-P-OP2	-6.44	99.91	105.70
2	S2	1022	U	C2-N1-C1'	6.40	125.38	117.70
25	SG	57	ASP	CB-CG-OD1	6.33	124.00	118.30
2	S2	427	U	N3-C2-O2	-6.29	117.80	122.20
2	S2	659	G	C4-N9-C1'	6.24	134.60	126.50
2	S2	1292	C	N1-C2-O2	6.21	122.63	118.90
2	S2	844	U	N1-C2-N3	6.21	118.62	114.90
2	S2	1520	G	C8-N9-C1'	-6.17	118.98	127.00
2	S2	1016	U	N3-C2-O2	-6.16	117.89	122.20
2	S2	1520	G	N3-C4-N9	6.15	129.69	126.00
2	S2	1453	C	C6-N1-C2	-6.07	117.87	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	S2	844	U	C2-N3-C4	-6.06	123.36	127.00
2	S2	1315	U	N1-C2-O2	6.03	127.02	122.80
2	S2	1729	U	N3-C2-O2	-6.02	117.99	122.20
7	SF	26	ASP	CB-CG-OD1	5.96	123.66	118.30
2	S2	501	C	C5-C6-N1	5.94	123.97	121.00
2	S2	1453	C	C5-C6-N1	5.93	123.97	121.00
2	S2	1520	G	N3-C4-C5	-5.93	125.63	128.60
2	S2	1118	C	N1-C2-O2	5.91	122.45	118.90
2	S2	537	C	C5-C6-N1	5.88	123.94	121.00
2	S2	1776	G	C4-N9-C1'	5.86	134.12	126.50
2	S2	1756	C	C6-N1-C1'	5.86	127.83	120.80
2	S2	1173	A	C6-N1-C2	-5.86	115.09	118.60
2	S2	118	C	C6-N1-C1'	-5.82	113.82	120.80
2	S2	195	C	C6-N1-C2	-5.82	117.97	120.30
2	S2	204	G	N1-C6-O6	-5.81	116.42	119.90
2	S2	293	C	C6-N1-C2	-5.80	117.98	120.30
2	S2	1389	C	C6-N1-C2	-5.79	117.98	120.30
2	S2	1660	C	C2-N1-C1'	5.77	125.15	118.80
2	S2	1271	C	C2-N1-C1'	5.76	125.14	118.80
2	S2	1415	C	C2-N1-C1'	5.76	125.13	118.80
2	S2	293	C	C5-C6-N1	5.73	123.86	121.00
2	S2	194	C	N1-C2-O2	5.72	122.33	118.90
6	SE	139	LEU	CA-CB-CG	5.70	128.41	115.30
2	S2	1777	G	C5-C6-O6	5.68	132.01	128.60
2	S2	1471	C	N1-C2-O2	5.57	122.24	118.90
2	S2	1660	C	N1-C2-O2	5.57	122.24	118.90
2	S2	1261	C	N1-C2-O2	5.55	122.23	118.90
2	S2	882	U	C5-C6-N1	5.55	125.48	122.70
2	S2	427	U	N1-C2-O2	5.54	126.68	122.80
2	S2	1756	C	N1-C2-N3	5.52	123.06	119.20
2	S2	466	G	C4-N9-C1'	5.51	133.66	126.50
2	S2	585	C	C2-N1-C1'	5.50	124.85	118.80
2	S2	1315	U	N3-C2-O2	-5.50	118.35	122.20
2	S2	205	G	N1-C2-N2	-5.49	111.26	116.20
2	S2	1315	U	C2-N1-C1'	5.48	124.28	117.70
2	S2	1123	C	C2-N1-C1'	5.48	124.82	118.80
2	S2	532	C	N3-C2-O2	-5.47	118.07	121.90
2	S2	1123	C	N1-C2-O2	5.47	122.18	118.90
2	S2	1777	G	N1-C2-N2	-5.44	111.30	116.20
2	S2	325	C	C2-N1-C1'	5.44	124.78	118.80
2	S2	659	G	C8-N9-C1'	-5.43	119.94	127.00
2	S2	4	C	C2-N1-C1'	5.43	124.77	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	S2	882	U	C6-N1-C2	-5.42	117.75	121.00
2	S2	1827	U	N1-C2-O2	5.41	126.58	122.80
2	S2	1660	C	N3-C2-O2	-5.39	118.13	121.90
2	S2	112	U	P-O3'-C3'	5.38	126.16	119.70
2	S2	882	U	C5-C4-O4	5.36	129.12	125.90
2	S2	1776	G	C8-N9-C1'	-5.35	120.05	127.00
3	SA	8	LEU	CA-CB-CG	5.35	127.60	115.30
2	S2	579	C	N1-C2-O2	5.35	122.11	118.90
2	S2	1739	C	C2-N1-C1'	5.34	124.68	118.80
2	S2	325	C	N1-C2-O2	5.33	122.10	118.90
35	Sf	103	LEU	CA-CB-CG	5.33	127.56	115.30
2	S2	1116	C	N1-C2-O2	5.30	122.08	118.90
2	S2	1471	C	C2-N1-C1'	5.27	124.60	118.80
2	S2	1434	C	P-O3'-C3'	5.25	126.00	119.70
2	S2	49	C	N3-C2-O2	-5.25	118.23	121.90
2	S2	1827	U	C2-N1-C1'	5.23	123.98	117.70
2	S2	1415	C	C5-C6-N1	5.22	123.61	121.00
2	S2	466	G	C8-N9-C1'	-5.19	120.25	127.00
28	SN	32	ASP	CB-CG-OD1	5.19	122.97	118.30
2	S2	580	U	N3-C2-O2	-5.18	118.57	122.20
2	S2	1415	C	N1-C2-O2	5.18	122.01	118.90
2	S2	1271	C	N3-C2-O2	-5.18	118.28	121.90
2	S2	1292	C	N3-C2-O2	-5.18	118.28	121.90
2	S2	291	G	P-O3'-C3'	5.17	125.90	119.70
2	S2	494	C	N1-C2-O2	5.15	121.99	118.90
2	S2	1649	U	N1-C2-O2	5.15	126.40	122.80
5	SD	154	ASP	CB-CG-OD1	5.15	122.93	118.30
2	S2	841	G	N1-C2-N2	-5.14	111.57	116.20
2	S2	834	C	C6-N1-C2	-5.14	118.25	120.30
2	S2	1123	C	C6-N1-C2	-5.12	118.25	120.30
2	S2	1261	C	C2-N1-C1'	5.09	124.40	118.80
2	S2	1309	C	C5-C6-N1	5.09	123.54	121.00
2	S2	466	G	N3-C4-N9	5.07	129.04	126.00
2	S2	1777	G	N1-C6-O6	-5.04	116.88	119.90
2	S2	201	C	N1-C2-O2	5.02	121.91	118.90
5	SD	14	ASP	CB-CG-OD1	5.02	122.82	118.30
2	S2	1755	C	C6-N1-C1'	-5.02	114.78	120.80

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Ln	230	0	276	0	0
2	S2	36538	0	18415	291	0
3	SA	1741	0	1746	25	0
4	SB	1738	0	1809	19	0
5	SD	1765	0	1865	28	0
6	SE	2076	0	2177	28	0
7	SF	1495	0	1549	17	0
8	SH	1497	0	1590	52	0
9	SI	1686	0	1772	22	0
10	SK	827	0	854	9	0
11	SL	1247	0	1323	19	0
12	SP	985	0	1031	10	0
13	SQ	1142	0	1213	20	0
14	SR	1090	0	1149	6	0
15	SS	1198	0	1261	23	0
16	ST	1112	0	1146	19	0
17	SU	821	0	883	9	0
18	SV	636	0	637	13	0
19	SX	1098	0	1167	11	0
20	Sa	821	0	870	0	0
21	Sc	506	0	536	0	0
22	Sd	459	0	448	0	0
23	Sg	2436	0	2393	0	0
24	SC	1725	0	1813	25	0
25	SG	1923	0	2088	35	0
26	SJ	1525	0	1640	11	0
27	SM	940	0	965	11	0
28	SN	1208	0	1294	12	0
29	SO	1049	0	1073	18	0
30	SW	1034	0	1080	9	0
31	SY	1065	0	1142	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	SZ	598	0	656	9	0
33	Sb	651	0	672	0	0
34	Se	459	0	503	0	0
35	Sf	548	0	552	0	0
36	CD	346	0	334	7	0
37	S2	21	0	0	0	0
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	656	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 (656) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
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
13:SQ:48:GLN:C	13:SQ:50:LYS:H	1.98	0.66
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
2:S2:1091:C:HO2'	30:SW:2:VAL:N	1.94	0.65
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S2:1488:C:O2'	2:S2:1490:G:OP2	2.14	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
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
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
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
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
2:S2:420:G:O2'	2:S2:660:C:N3	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
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
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
27:SM:66:GLU:HG3	27:SM:76:LEU:HD21	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
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
2:S2:168:C:O2'	25:SG:133:LEU:O	2.22	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
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
2:S2:1764:G:H5'	2:S2:1765:C:H5"	1.88	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
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
2:S2:1758:G:C5	2:S2:1771:G:N2	2.75	0.55
13:SQ:43:GLU:HB3	13:SQ:44:PRO:HD2	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:SS:118:ARG:HE	15:SS:123:LEU:HD21	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:S2:1755: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:S2:1396:A:O2'	2:S2:1398:G:N7	2.33	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
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
2:S2:453:C:O2'	25:SG:92:ARG:O	2.22	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
11:SL:75:GLY:HA3	11:SL:88:ILE:HD12	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:SD:8:LYS:HG2	17:SU:61:LEU:HD11	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:S2:928:G:H2'	2:S2:929:G:C8	2.44	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
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
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:S2:156:G:OP1	25:SG:2:LYS:NZ	2.43	0.51
12:SP:64:LYS:NZ	12:SP:91:GLY:O	2.42	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
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
13:SQ:48:GLN:C	13:SQ:50:LYS:N	2.62	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
15:SS:16:LEU:HD21	15:SS:72:GLN:HE21	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:SV:30:ALA:O	18:SV:60:ARG:NH1	2.40	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
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
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
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
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
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
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
29:SO:14:VAL:H	29:SO:15:ILE:HA	1.77	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
25:SG:32:MET:HA	25:SG:52:ILE:HB	1.94	0.49
2:S2:367:U:H4'	2:S2:371:A:C8	2.48	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
4:SB:138:PHE:O	4:SB:213:ARG:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:S2:641: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
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
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
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
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
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
2:S2:1232:U:H2'	2:S2:1233:G:C8	2.48	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
36:CD:132:ASP:OD1	36:CD:132:ASP:N	2.44	0.48
25:SG:198:ARG:O	25:SG:202:ASN:ND2	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
2:S2:54:A:OP1	31:SY:111:LYS:NZ	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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:S2:902: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
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
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
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:S2:1854: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:S2:1562:C:H2'	2:S2:1563:G:H8	1.80	0.46
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
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
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
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:S2:907: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
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
31:SY:12:PHE:HZ	31:SY:21:LYS:HD2	1.81	0.46
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
16:ST:65:TYR:HE1	16:ST:128:GLN:HG3	1.81	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:S2:886: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
2:S2:104:A:OP1	9:SI:12:ARG:NH1	2.46	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:N	11:SL:3:ASP:OD1	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
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
2:S2:507:G:OP1	31:SY:108:LYS:NZ	2.37	0.44
13:SQ:86:GLN:HE22	13:SQ:122:ALA:HA	1.82	0.44
29:SO:78:ALA:HB3	29:SO:118:ALA:HB3	1.97	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:SI:101:ILE:HD12	9:SI:190:LEU:HD11	1.99	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:S2:5:U:OP2	24:SC:230:THR:OG1	2.31	0.44
24:SC:183:LYS:HG2	30:SW:95:PRO:HA	1.99	0.44
2:S2:604:A:N3	2:S2:639:C:O2'	2.45	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
25:SG:2:LYS:HB2	25:SG:108:VAL:HG23	1.98	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
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
2:S2:1589:A:N3	2:S2:1653:U:O2'	2.38	0.43
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
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
29:SO:57:THR:HG23	29:SO:60:MET:HE2	2.00	0.43
2:S2:1:U:O2	2:S2:3:C:C4	2.72	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
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
3:SA:37:TYR:OH	3:SA:57:LYS:NZ	2.52	0.43
7:SF:124:ASP:N	7:SF:124:ASP:OD1	4.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:SA:51:LEU:HA	3:SA:54:THR:HG22	2.01	0.43
32:SZ:43:LYS:O	32:SZ:44:LEU:C	2.57	0.43
3:SA:206:ASP:N	3:SA:206:ASP:OD1	2.51	0.43
15:SS:13:LEU:HB2	15:SS:20:ILE:HG12	2.00	0.43
27:SM:53:ALA:O	27:SM:78:LYS:NZ	2.50	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
5:SD:22:ASN:O	5:SD:26:THR:OG1	2.31	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
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
3:SA:76:VAL:HG12	3:SA:123:VAL:HB	2.01	0.43
24:SC:113:GLN:HE21	24:SC:120:GLN:HG3	1.84	0.43
2:S2:126:G:OP2	25:SG:195:LYS:NZ	2.36	0.42
5:SD:158:ILE:HG13	5:SD:164:VAL:HG12	2.00	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
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:S2:1734: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
4:SB:178:THR:HG23	4:SB:179:ASN:ND2	2.35	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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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
2:S2:570:C:O2'	31:SY:34:THR:O	2.27	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
18:SV:47:ASN:N	18:SV:47:ASN:OD1	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
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
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
6:SE:41:CYS:HA	6:SE:85:GLY:HA2	2.03	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
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
17:SU:46:LYS:HZ1	17:SU:101:ILE:HD11	1.85	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
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:S2:1622: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:SE:51:ARG:NH1	6:SE:109:PHE:O	2.53	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
2:S2:25:A:HO2'	2:S2:26:U:H6	1.69	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

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%)	29	61
4	SB	212/264 (80%)	195 (92%)	15 (7%)	2 (1%)	17	48
5	SD	225/243 (93%)	214 (95%)	10 (4%)	1 (0%)	34	66
6	SE	260/263 (99%)	253 (97%)	7 (3%)	0	100	100
7	SF	187/204 (92%)	172 (92%)	14 (8%)	1 (0%)	29	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
8	SH	182/194 (94%)	158 (87%)	22 (12%)	2 (1%)	14 42
9	SI	204/208 (98%)	189 (93%)	14 (7%)	1 (0%)	29 61
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%)	7 26
14	SR	133/135 (98%)	125 (94%)	7 (5%)	1 (1%)	19 51
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%)	22 54
20	Sa	100/115 (87%)	93 (93%)	6 (6%)	1 (1%)	15 45
21	Sc	62/69 (90%)	51 (82%)	9 (14%)	2 (3%)	4 16
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%)	34 66
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%)	22 54
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%)	2 5
33	Sb	81/84 (96%)	72 (89%)	9 (11%)	0	100 100
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%)	38 66

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 (i)

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%)	194 (100%)	1 (0%)	88 96
5	SD	190/202 (94%)	189 (100%)	1 (0%)	88 96
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%)	160 (96%)	6 (4%)	35 69
9	SI	178/180 (99%)	178 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	SK	89/136 (65%)	88 (99%)	1 (1%)	73 92
11	SL	137/142 (96%)	135 (98%)	2 (2%)	65 87
12	SP	107/130 (82%)	107 (100%)	0	100 100
13	SQ	119/121 (98%)	113 (95%)	6 (5%)	24 57
14	SR	122/122 (100%)	122 (100%)	0	100 100
15	SS	126/132 (96%)	125 (99%)	1 (1%)	81 94
16	ST	113/115 (98%)	112 (99%)	1 (1%)	78 93
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%)	112 (99%)	1 (1%)	78 93
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%)	30 63
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%)	206 (100%)	1 (0%)	88 96
26	SJ	161/168 (96%)	161 (100%)	0	100 100
27	SM	102/108 (94%)	99 (97%)	3 (3%)	42 76
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%)	112 (99%)	1 (1%)	78 93
32	SZ	66/103 (64%)	60 (91%)	6 (9%)	9 28
33	Sb	75/76 (99%)	75 (100%)	0	100 100
34	Se	47/48 (98%)	47 (100%)	0	100 100
35	Sf	60/140 (43%)	59 (98%)	1 (2%)	60 86
36	CD	35/404 (9%)	35 (100%)	0	100 100
All	All	4277/5088 (84%)	4243 (99%)	34 (1%)	82 94

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	SB	51	ARG

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Mol	Chain	Res	Type
5	SD	76	ARG
8	SH	9	VAL
8	SH	25	GLN
8	SH	27	LEU
8	SH	29	GLU
8	SH	43	LEU
8	SH	85	LYS
10	SK	95	ARG
11	SL	39	ASN
11	SL	69	ARG
13	SQ	10	VAL
13	SQ	39	LEU
13	SQ	41	MET
13	SQ	42	ILE
13	SQ	46	THR
13	SQ	48	GLN
15	SS	5	ILE
16	ST	41	LYS
19	SX	123	VAL
22	Sd	26	ASN
22	Sd	27	ARG
25	SG	119	LYS
27	SM	33	ARG
27	SM	63	LYS
27	SM	121	LYS
31	SY	132	LYS
32	SZ	42	ASP
32	SZ	44	LEU
32	SZ	50	PHE
32	SZ	51	ASP
32	SZ	79	ILE
32	SZ	83	LEU
35	Sf	89	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
4	SB	40	ASN
5	SD	56	GLN
6	SE	197	ASN
7	SF	31	ASN
8	SH	12	ASN

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Mol	Chain	Res	Type
11	SL	39	ASN
12	SP	98	ASN
15	SS	72	GLN
15	SS	87	GLN
17	SU	81	GLN
21	Sc	26	GLN
32	SZ	45	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	S2	1701/1869 (91%)	378 (22%)	4 (0%)

All (378) 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
2	S2	127	C

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Mol	Chain	Res	Type
2	S2	139	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	1771	G
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

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Mol	Chain	Res	Type
2	S2	1822	A
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 monosaccharides 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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

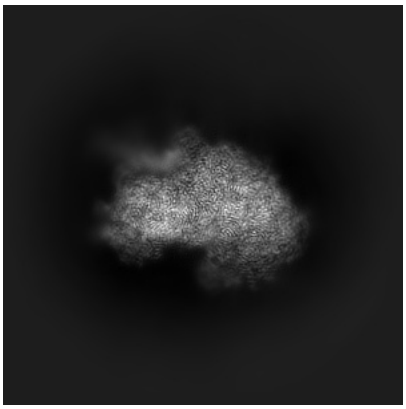
6 Map visualisation

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.

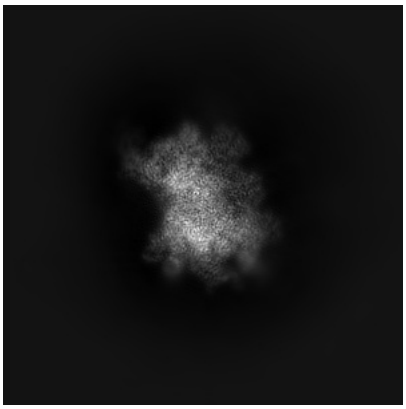
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

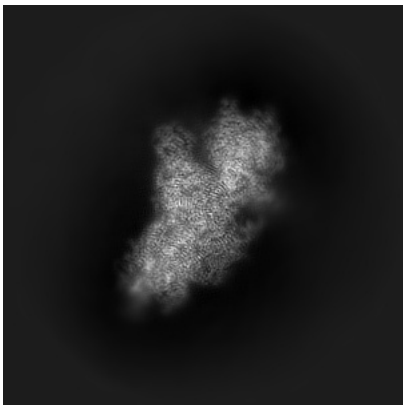
6.1.1 Primary map



X

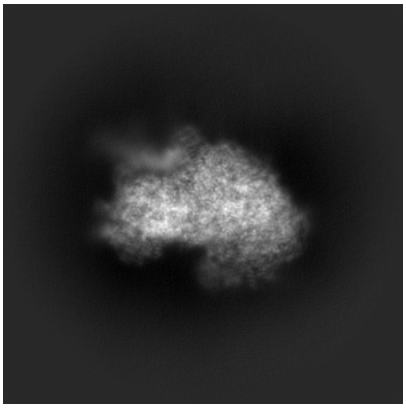


Y

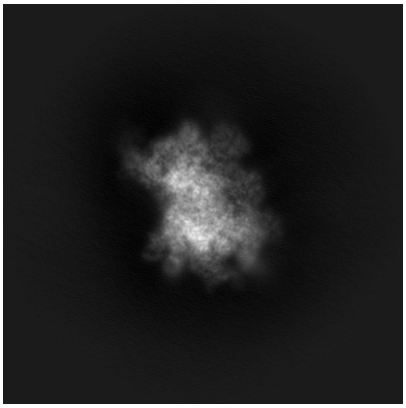


Z

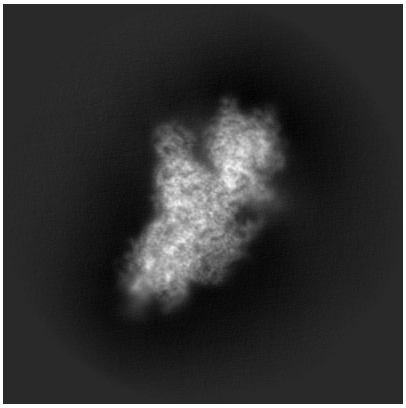
6.1.2 Raw map



X



Y



Z

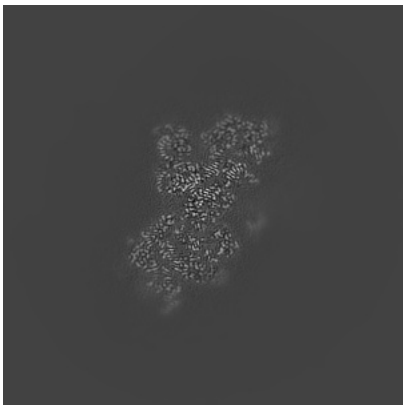
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map

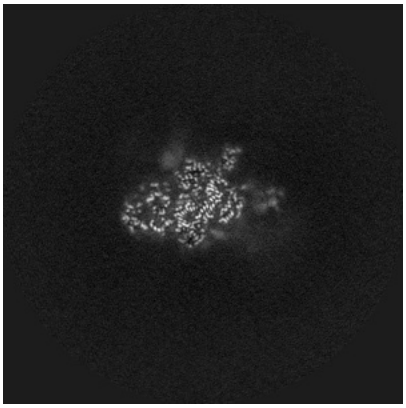
X Index: 210

Y Index: 210

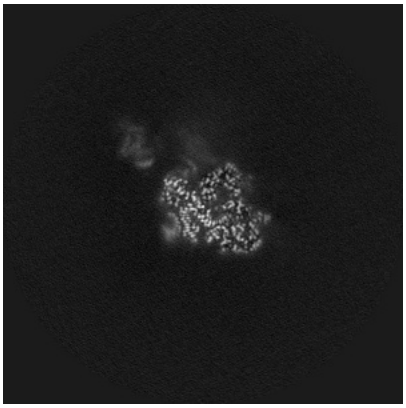


Z Index: 210

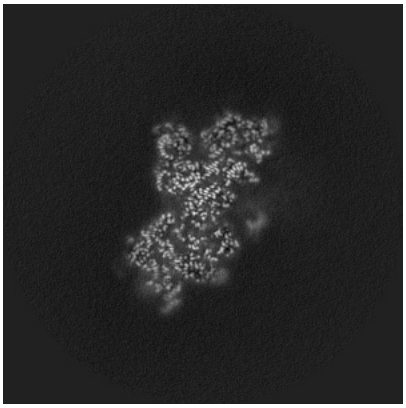
6.2.2 Raw map



X Index: 210



Y Index: 210

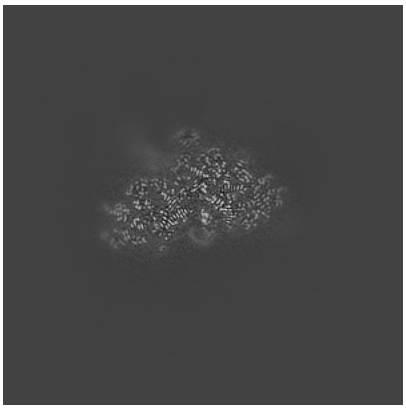


Z Index: 210

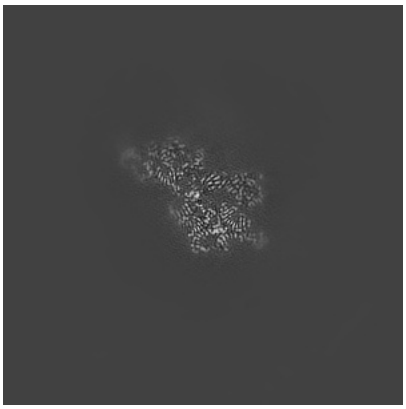
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

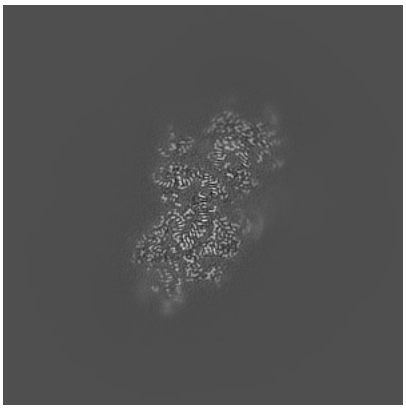
6.3.1 Primary map



X Index: 185

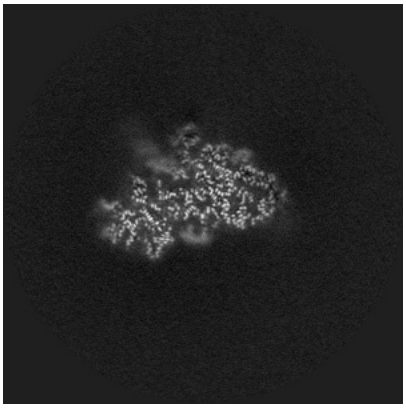


Y Index: 233

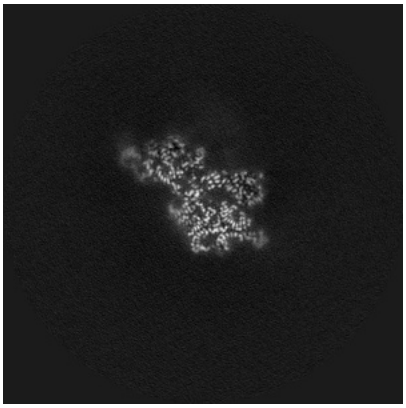


Z Index: 204

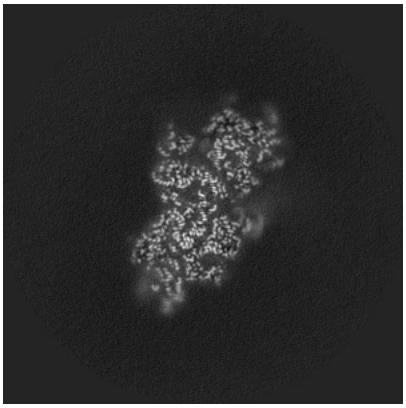
6.3.2 Raw map



X Index: 179



Y Index: 233

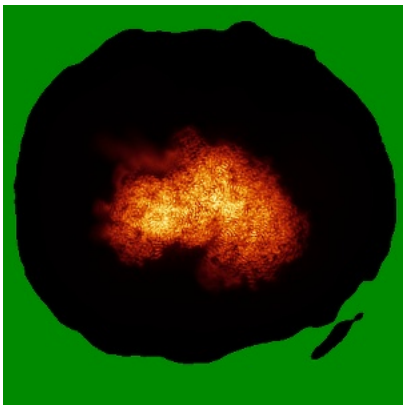


Z Index: 204

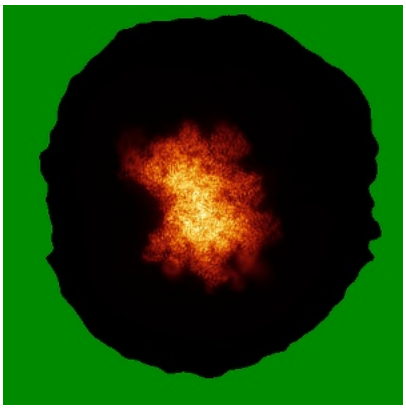
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

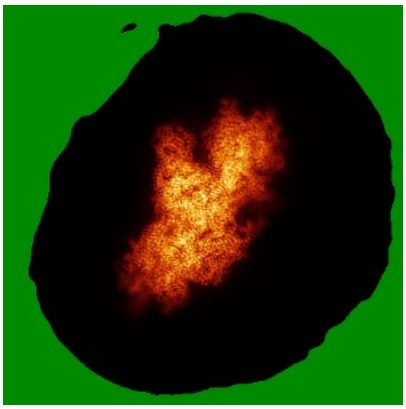
6.4.1 Primary map



X

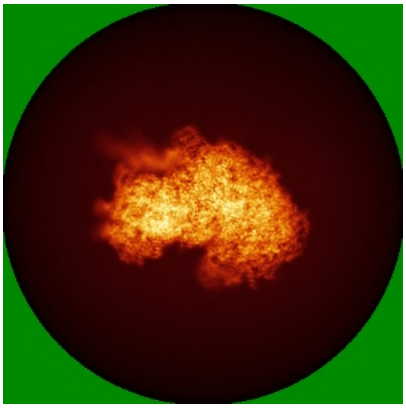


Y

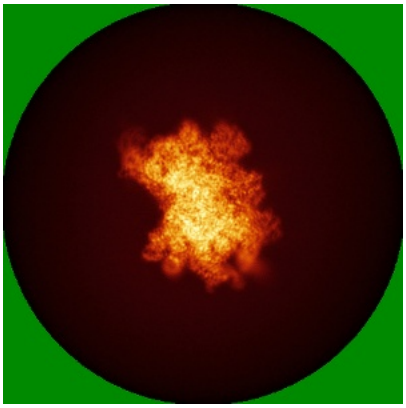


Z

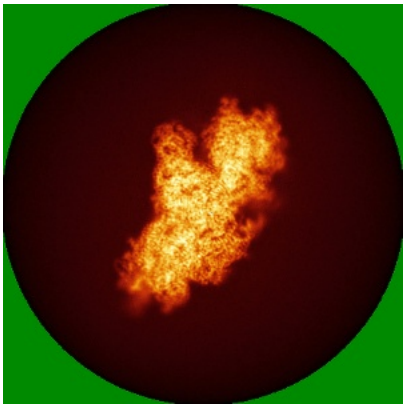
6.4.2 Raw map



X



Y

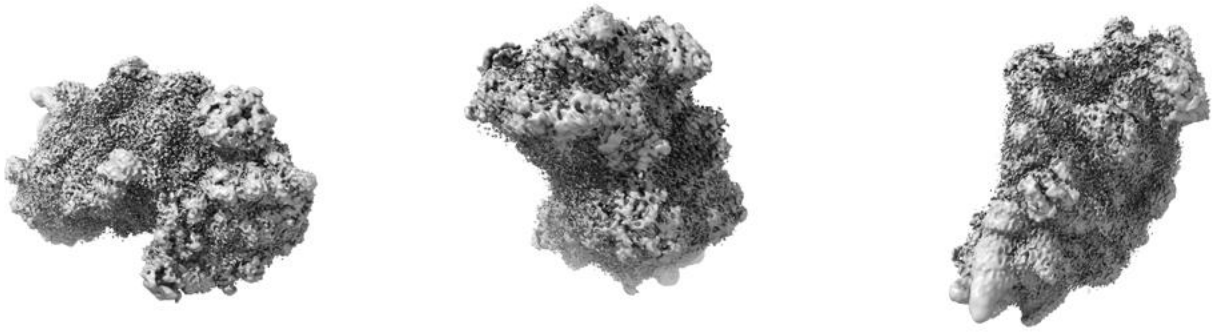


Z

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)

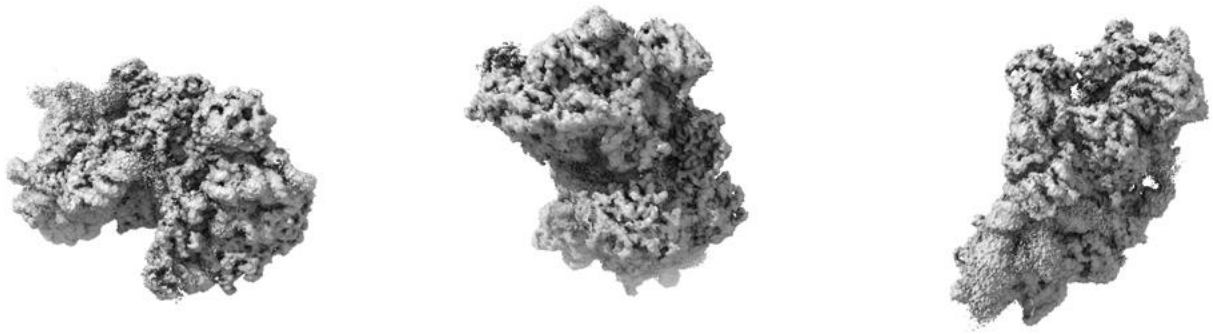
6.5.1 Primary map



X Y Z

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



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.

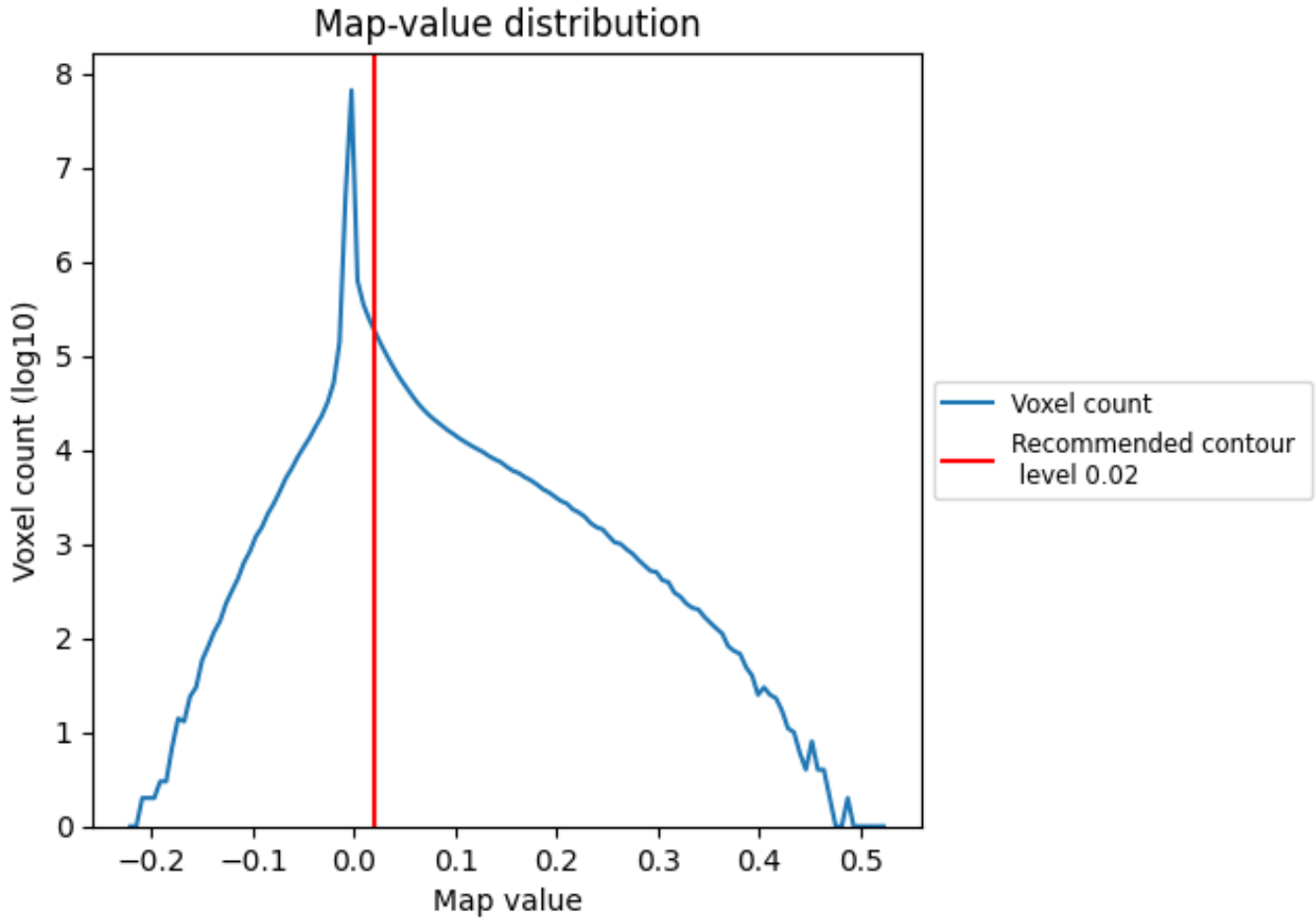
6.6 Mask visualisation (i)

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

7 Map analysis

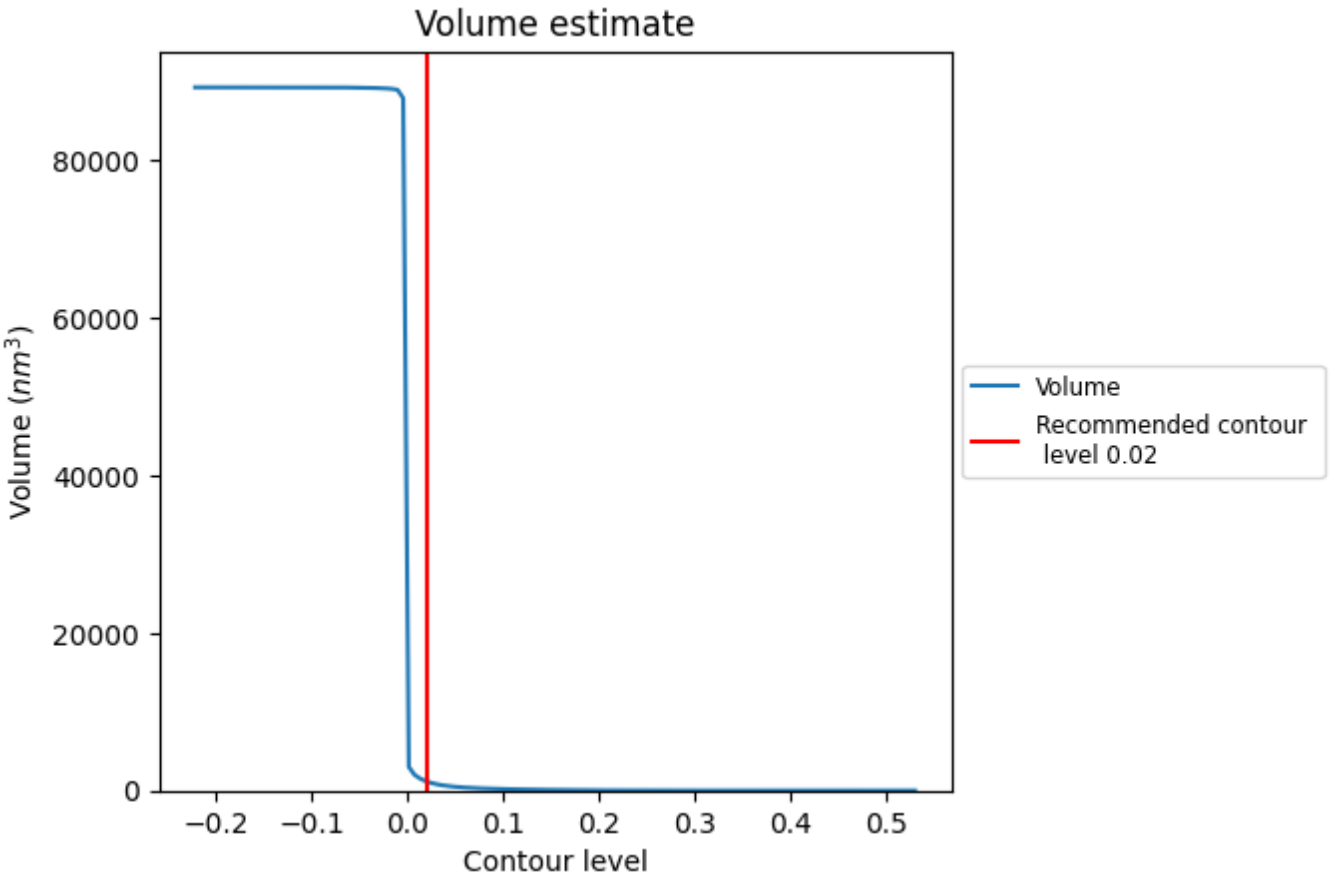
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

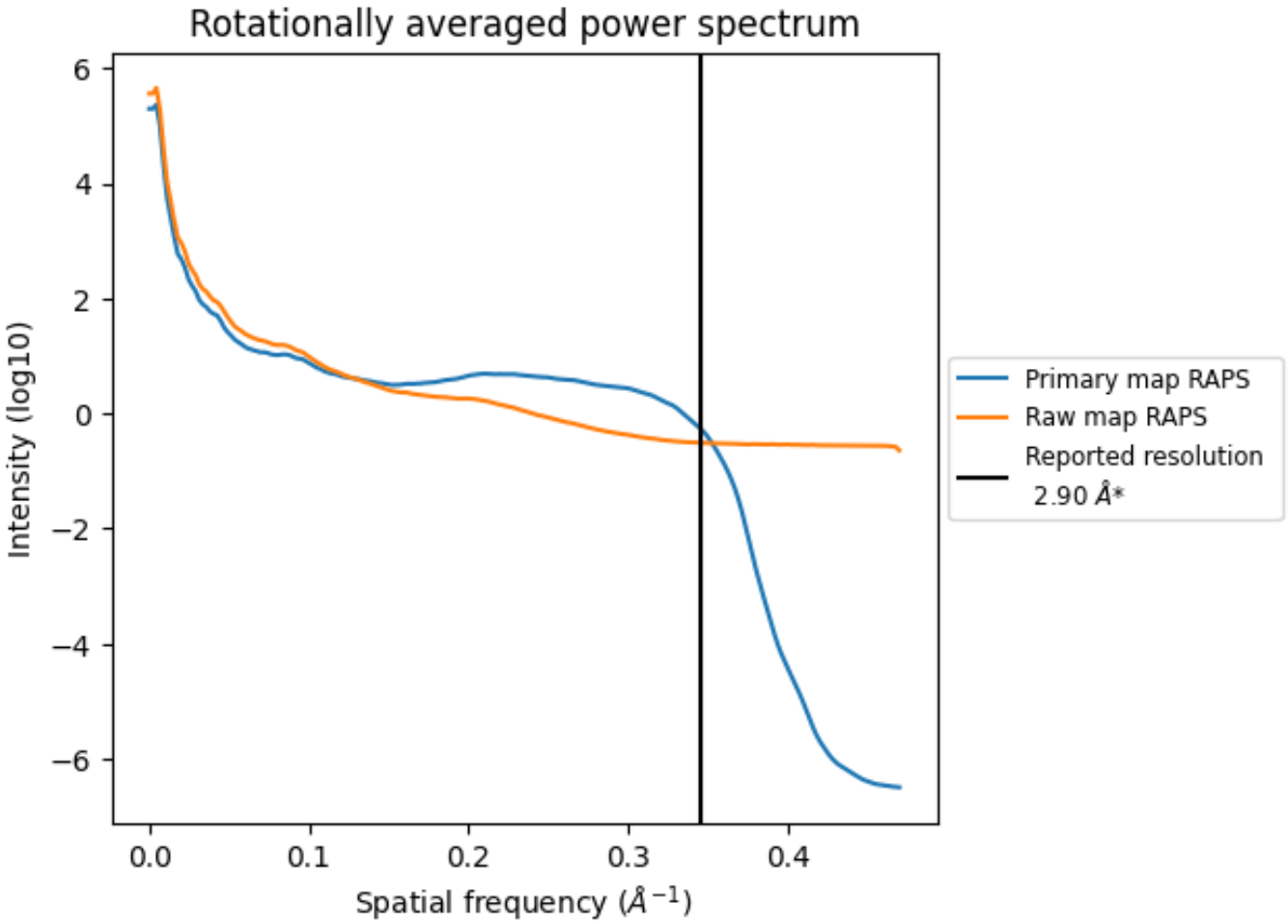
7.2 Volume estimate



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 (i)

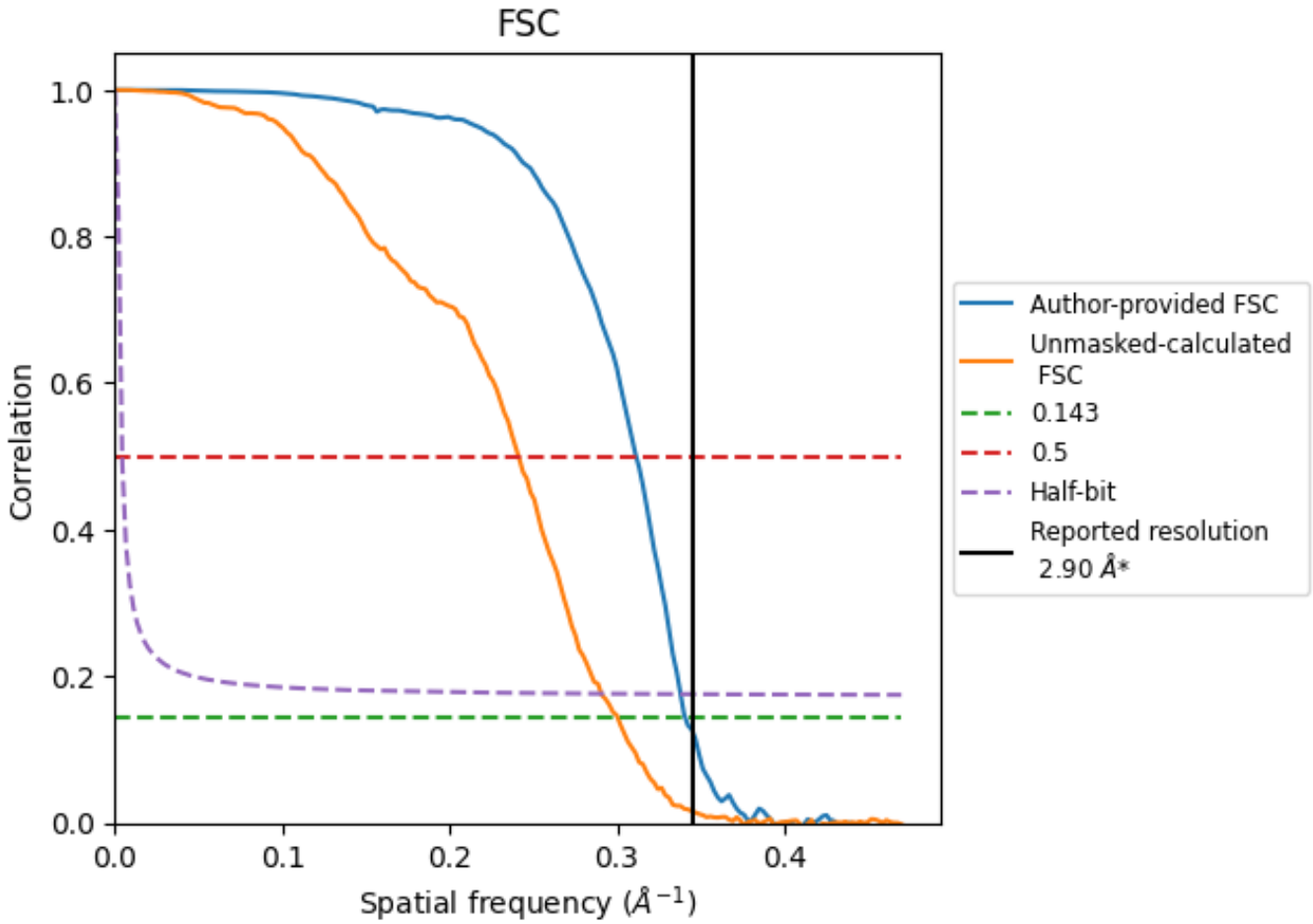


*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8.2 Resolution estimates (i)

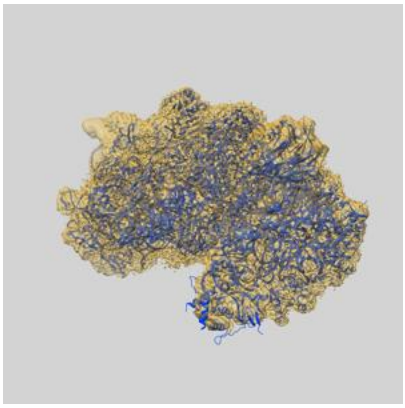
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.93	3.21	2.96
Unmasked-calculated*	3.33	4.15	3.44

*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 %

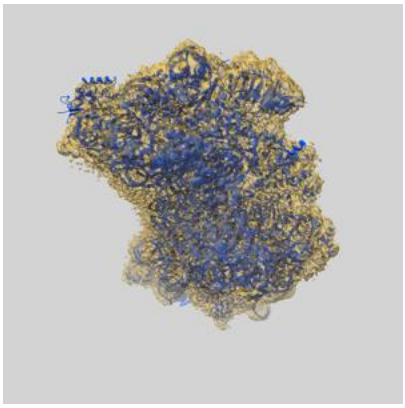
9 Map-model fit

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.

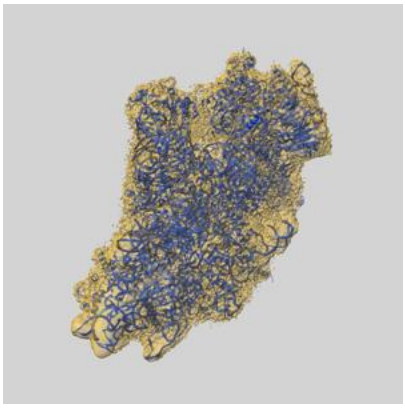
9.1 Map-model overlay



X



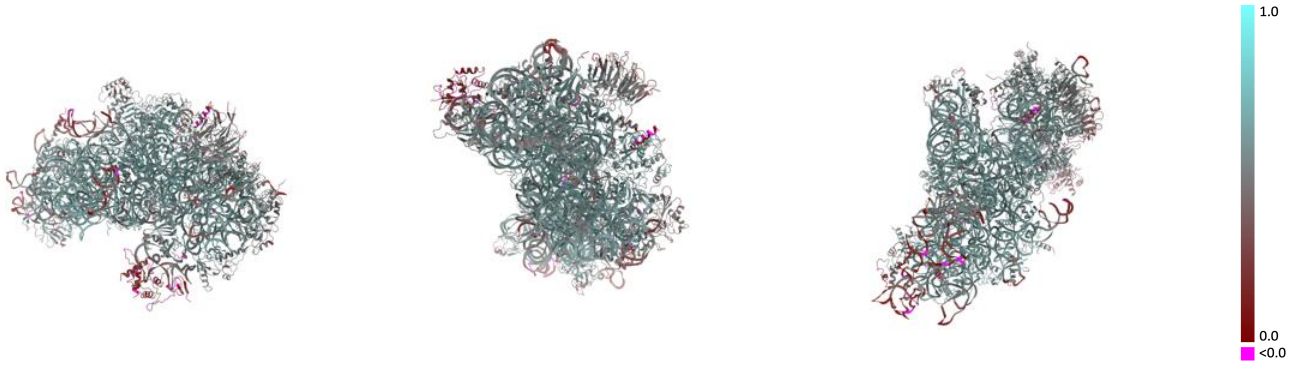
Y



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.

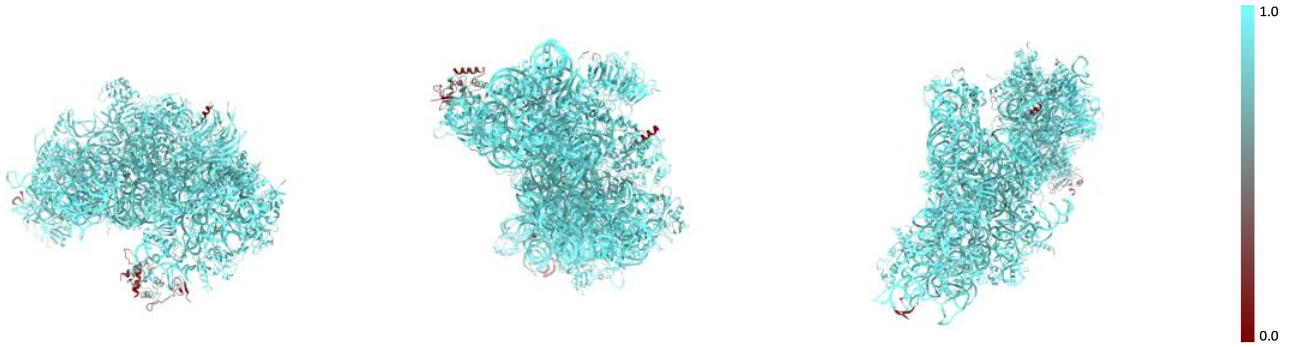
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

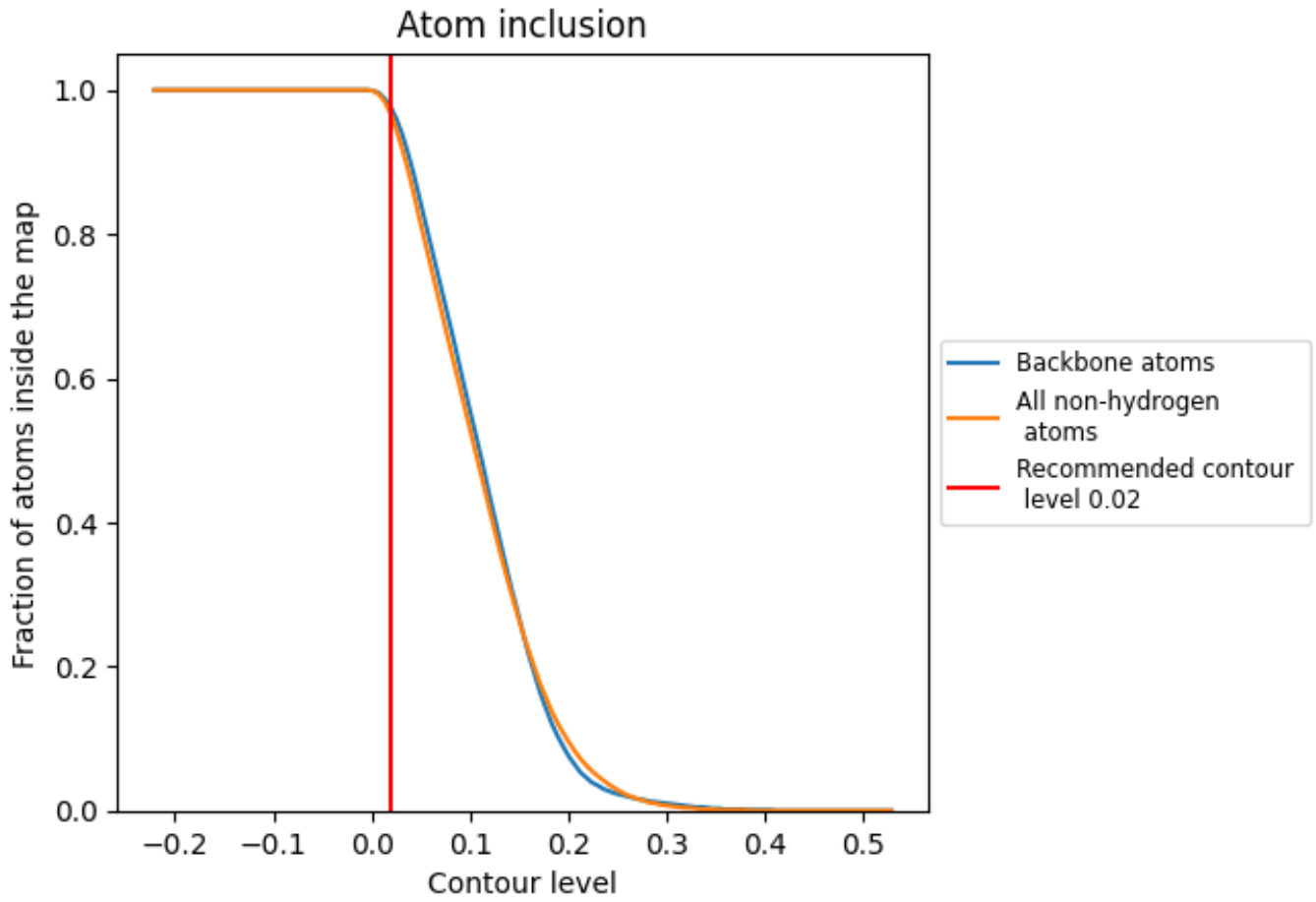
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (i)



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

Continued on next page...

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