



Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 03:31 AM UTC

PDB ID : 8XP2 / pdb_00008xp2
EMDB ID : EMD-38548
Title : Cryo-EM structure of the human 40S ribosome with LARP1
Authors : Huang, Z.; Ye, X.; Li, Y.; Cheng, J.
Deposited on : 2024-01-02
Resolution : 3.20 Å(reported)
Based on initial model : 6Z6M

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

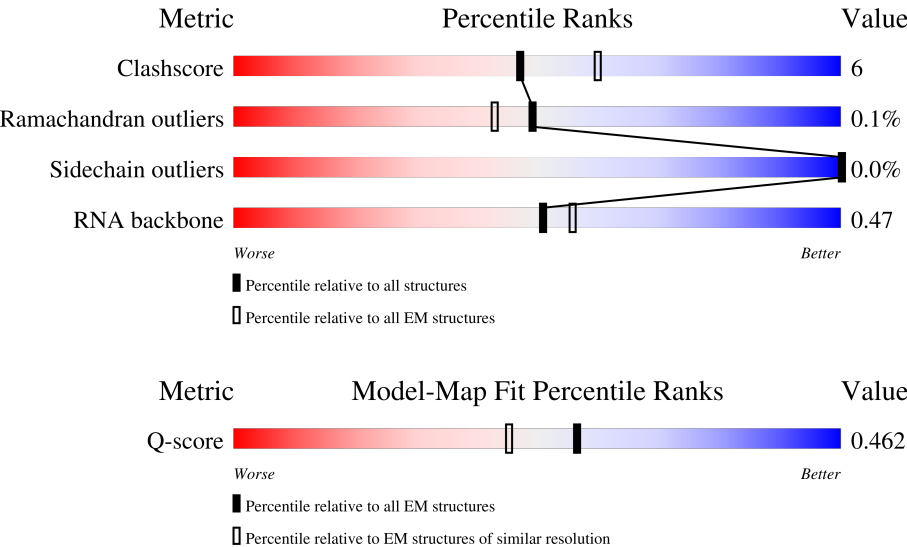
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 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.



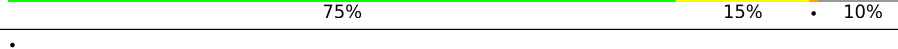
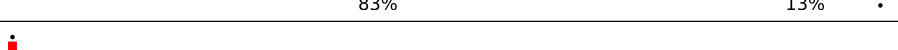
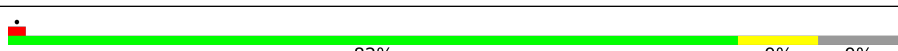
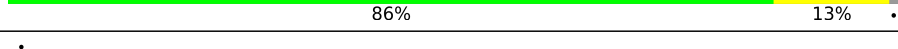
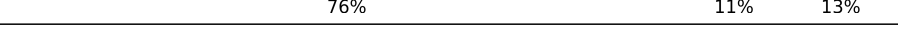
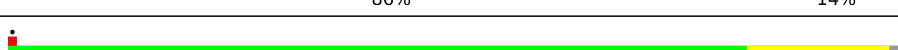
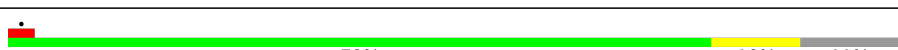
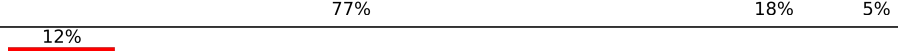
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	

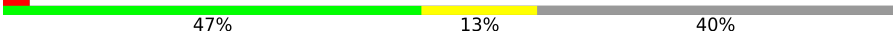
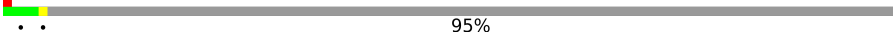
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Mol	Chain	Length	Quality of chain
4	SB	264	
5	SD	243	
6	SE	263	
7	SF	204	
8	SH	194	
9	SI	208	
10	SK	165	
11	SL	158	
12	SP	145	
13	SQ	146	
14	SR	135	
15	SS	152	
16	ST	145	
17	SU	119	
18	SV	83	
19	SX	143	
20	Sa	115	
21	Sc	69	
22	Sd	56	
23	Sg	317	
24	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	 80%9%11%
30	SW	130	 82%17%
31	SY	133	 73%21%6%
32	SZ	125	 47%13%40%
33	Sb	84	 85%14%
34	Se	59	 7%92%7%
35	Sf	156	 32%7%61%
36	JD	1096	 95%

2 Entry composition [i](#)

There are 37 unique types of molecules in this entry. The entry contains 76494 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	1740	Total	C	N	O	P	0	0
			36896	16458	6597	12102	1739		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S2	582	C	U	conflict	GB 36162
S2	583	C	A	conflict	GB 36162
S2	584	G	A	conflict	GB 36162
S2	798	A	G	conflict	GB 36162
S2	1095	U	C	conflict	GB 36162

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	SA	222	Total	C	N	O	S	0	0
			1747	1109	306	324	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	184	Total	C	N	O	S	0	0
			1461	914	276	264	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	144	Total	C	N	O	S	0	0
			1182	752	224	200	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	SP	127	Total	C	N	O	S	0	0
			1045	663	198	177	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	135	Total	C	N	O	S	0	0
			1010	618	198	188	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	125	Total	C	N	O	S	0	0
			1022	645	200	172	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	61	Total	C	N	O	S	0	0
			497	312	94	84	7		

- Molecule 36 is a protein called La-related protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	JD	52	Total	C	N	O	S	0	0
			429	269	75	83	2		

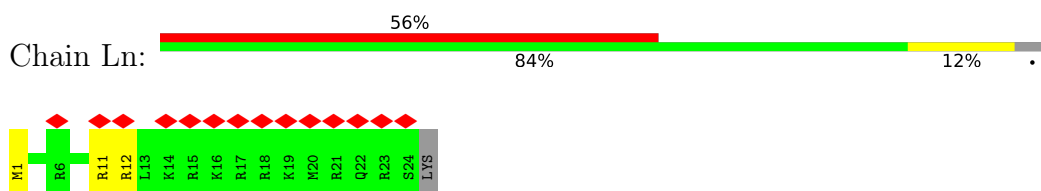
- Molecule 37 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

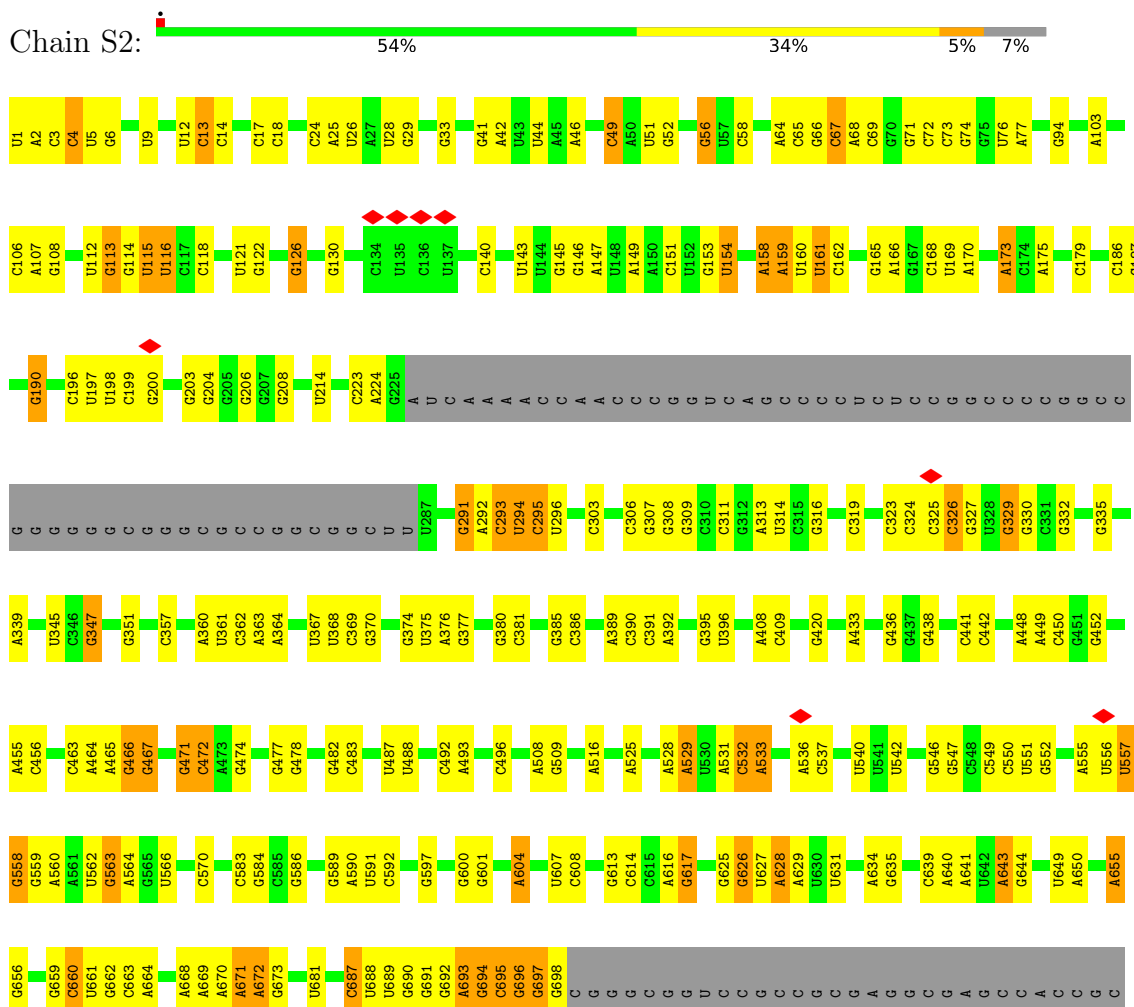
3 Residue-property plots

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.

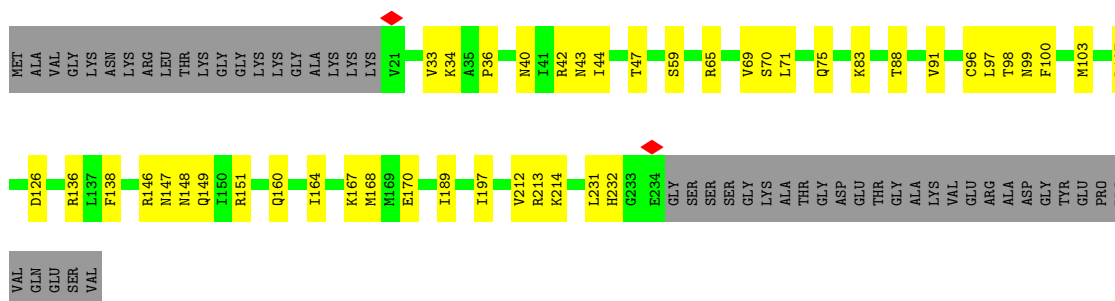
- Molecule 1: 60S ribosomal protein L41



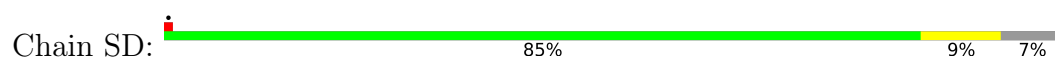
- Molecule 2: 18S rRNA



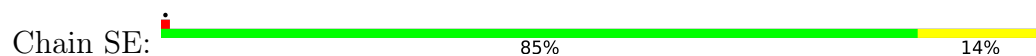
- Molecule 4: 40S ribosomal protein S3a



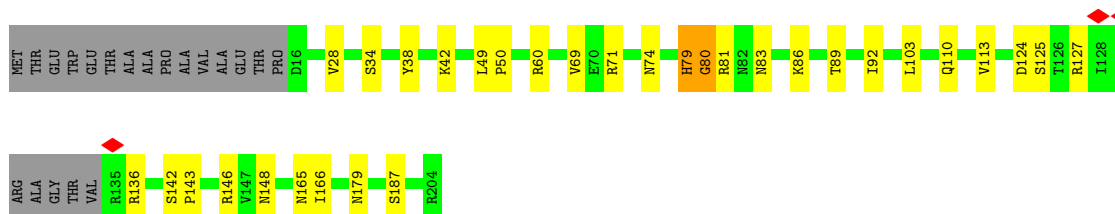
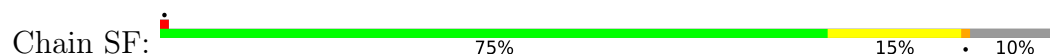
- Molecule 5: 40S ribosomal protein S3



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



- Molecule 7: 40S ribosomal protein S5



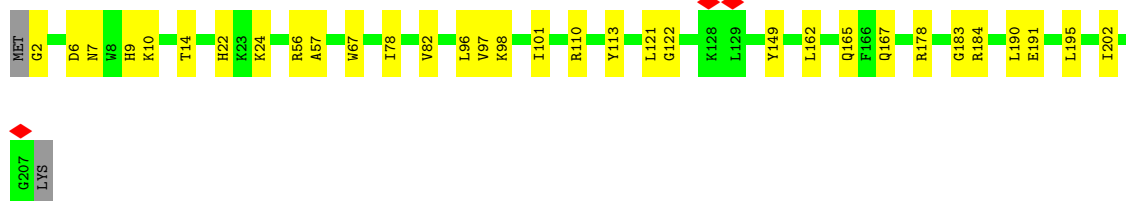
- Molecule 8: 40S ribosomal protein S7

Chain SH:  83% 13% .



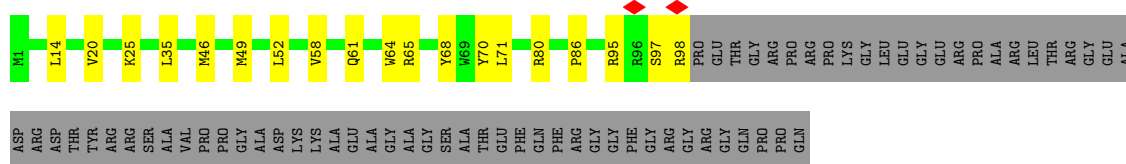
- Molecule 9: 40S ribosomal protein S8

Chain SI:  84% 15% .



- Molecule 10: 40S ribosomal protein S10

Chain SK:  48% 12% 41%



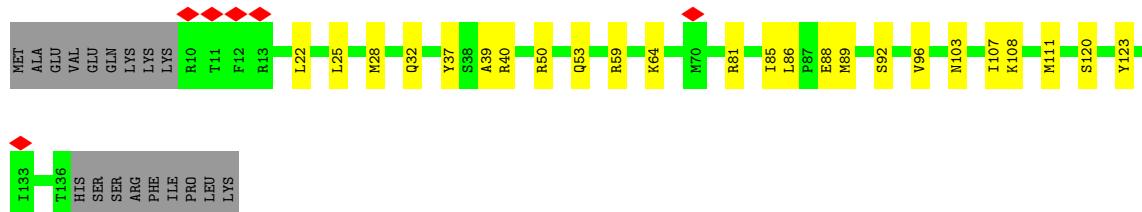
- Molecule 11: 40S ribosomal protein S11

Chain SL:  82% 9% 9%



- Molecule 12: 40S ribosomal protein S15

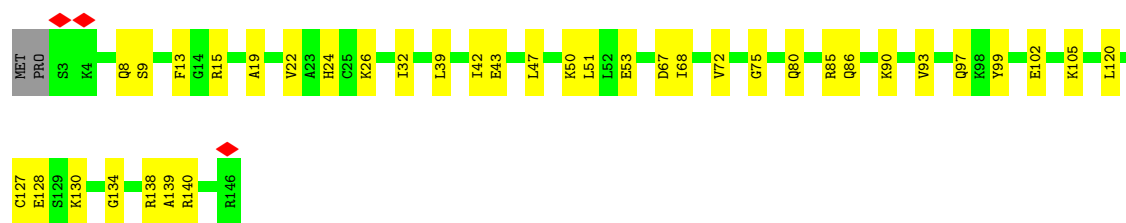
Chain SP:  71% 17% 12%



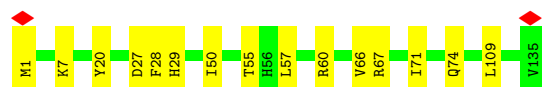
- Molecule 13: 40S ribosomal protein S16

Chain SQ:  73% 25% .

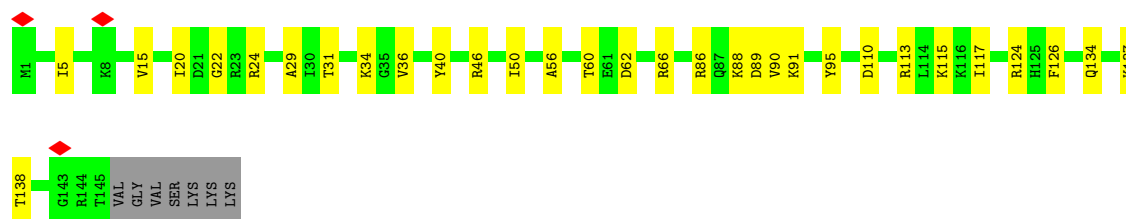
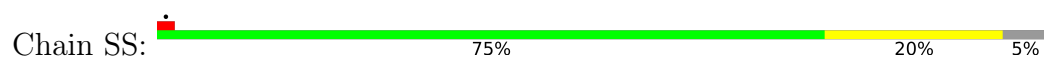




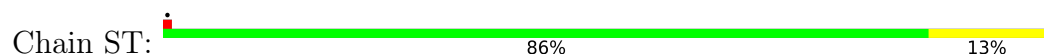
- Molecule 14: 40S ribosomal protein S17



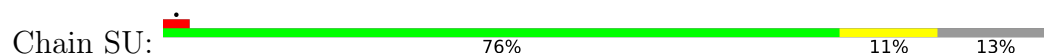
- Molecule 15: 40S ribosomal protein S18



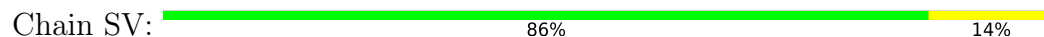
- Molecule 16: 40S ribosomal protein S19



- Molecule 17: 40S ribosomal protein S20



- Molecule 18: 40S ribosomal protein S21



- Molecule 19: 40S ribosomal protein S23

MET	G2	K3	T9	R17	H46	A47	K48	V51	K60	R67	K68	V72	L91	D98	A103	G104	D114	I115	F120	K124	V125	S129	Y134	R140	P141	R142	SER
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- MET T2 N7 A11 K12 C23 R28 D33 R85 Y66 R87 A91 P98 P99 R100 F101 R102 R103 ALA GLY PRO ARG PRO PRO PRO LYS MET
-

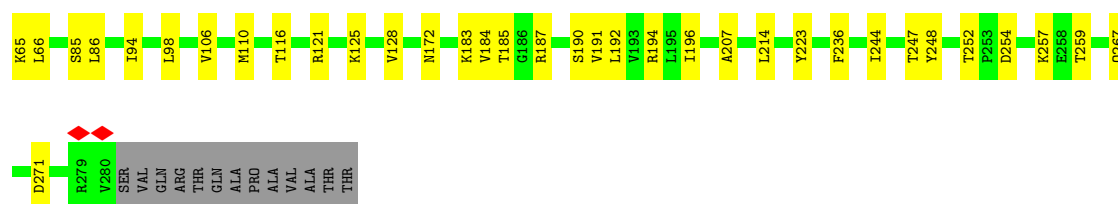
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- Sequence logo for the 1000bp upstream region of the R67 gene. The y-axis represents information content in bits (0.00 to 0.15). The x-axis shows amino acid positions from MET to ARG. The sequence is MET ASP THR SER R5 R13 T21 Q29 F34 P49 V55 R67 L68 ARG. Red diamonds mark positions R5, R67, and L68. The R67 position shows the highest information content, with 'R' being the most conserved residue.

-
- | Category | Value |
|----------|-------|
| MET | 16 |
| G2 | 15 |
| H3 | 14 |
| Q4 | 13 |
| Q5 | 12 |
| L6 | 11 |
| S9 | 10 |
| R12 | 9 |
| C21 | 8 |
| N26 | 7 |
| R27 | 6 |
| F52 | 5 |
| D56 | 4 |

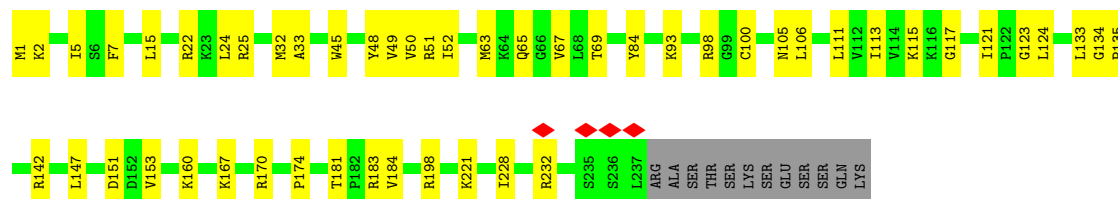
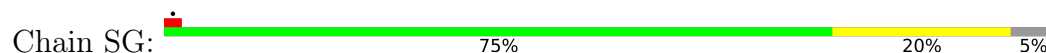
- | MET |
|-----|
| T2 |
| E3 |
| Q4 |
| M5 |
| R8 |
| G9 |
| T10 |
| L11 |
| H14 |
| W17 |
| T23 |
| Q26 |
| I31 |
| L32 |
| S33 |
| R36 |
| T39 |
| L40 |
| L45 |
| T46 |
| R47 |
| D48 |
| E49 |
| T50 |
| N51 |
| Y52 |
| G53 |
| R57 |
| A58 |
| L59 |
| R60 |
| G61 |
| H62 |
| V66 |
| S72 |
| S73 |
| D74 |
| S80 |
| X81 |
| S82 |
| L87 |
| L92 |
| C95 |

[illegible]

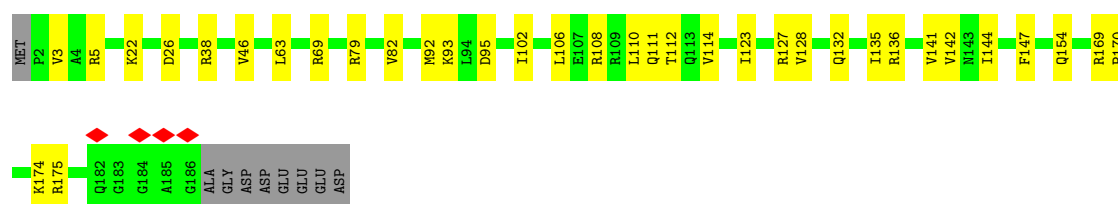
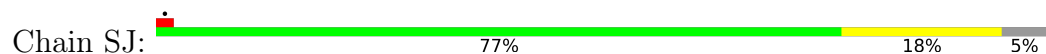
- [illegible]



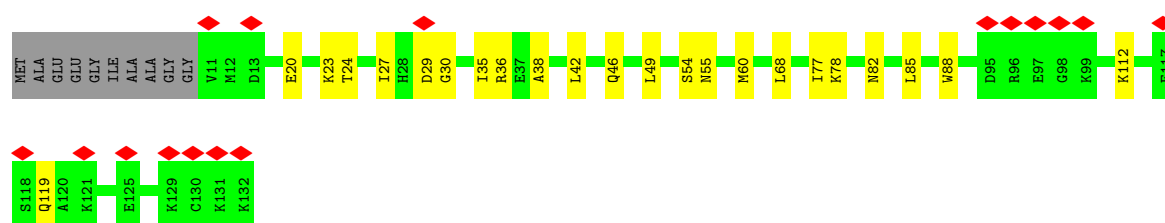
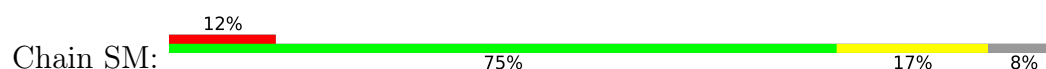
- Molecule 25: 40S ribosomal protein S6



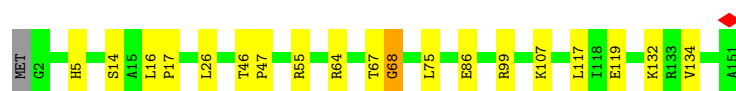
- Molecule 26: 40S ribosomal protein S9



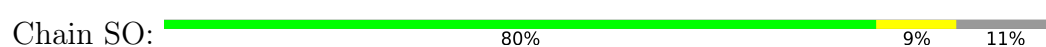
- Molecule 27: 40S ribosomal protein S12



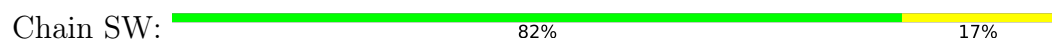
- Molecule 28: 40S ribosomal protein S13



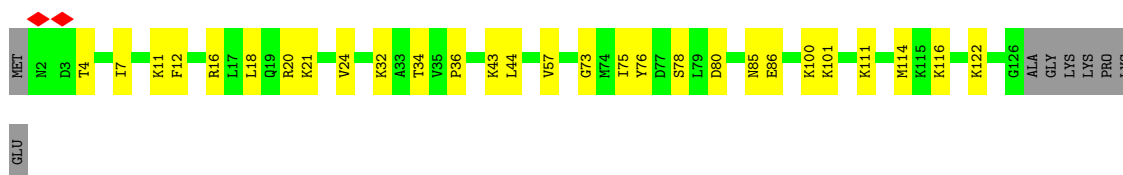
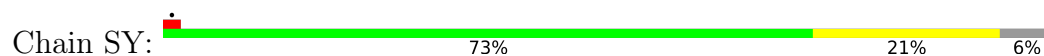
- Molecule 29: 40S ribosomal protein S14



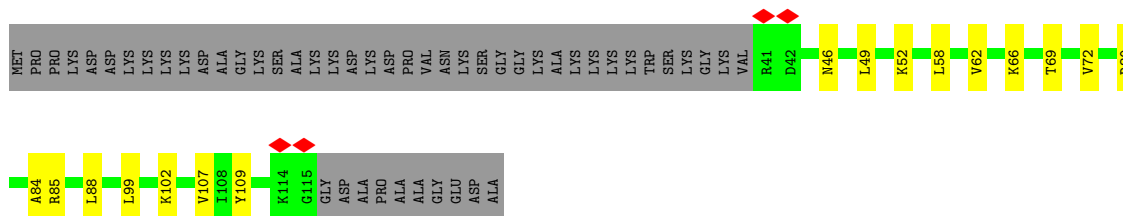
- Molecule 30: 40S ribosomal protein S15a



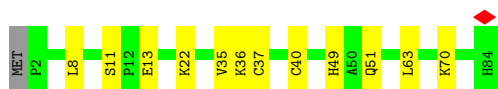
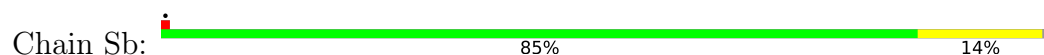
- Molecule 31: 40S ribosomal protein S24



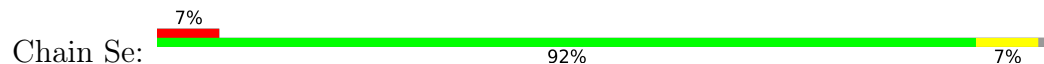
- Molecule 32: 40S ribosomal protein S25



- Molecule 33: 40S ribosomal protein S27



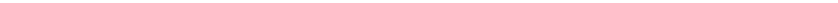
- Molecule 34: 40S ribosomal protein S30

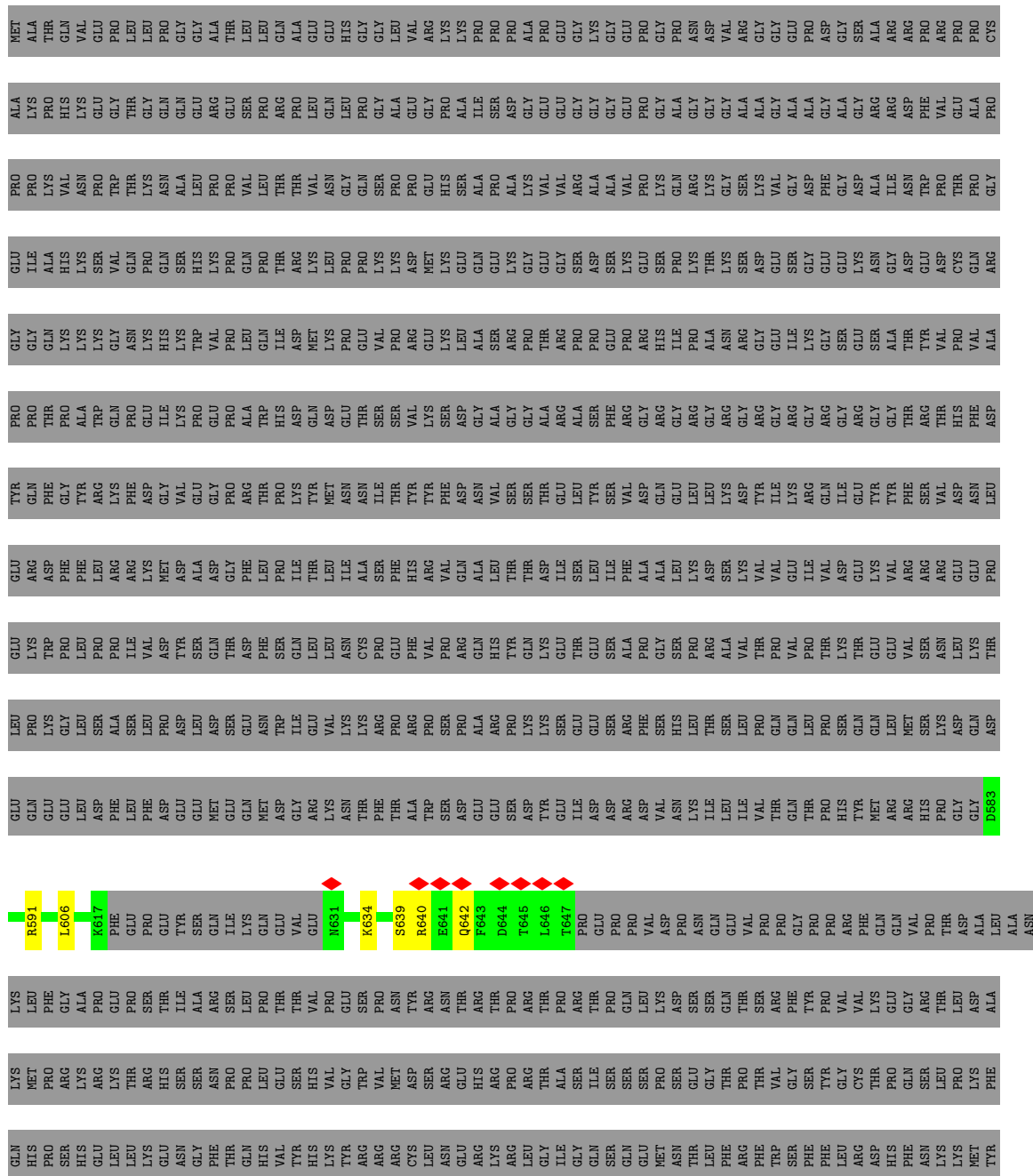


- Molecule 35: Ubiquitin-40S ribosomal protein S27a



- Molecule 36: La-related protein 1

Chain ID: 



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	25959	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Relion	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.077	Depositor
Minimum map value	-0.026	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	481.32, 481.32, 481.32	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.146, 1.146, 1.146	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Ln	0.08	0/231	0.30	0/294
2	S2	0.17	0/41241	0.35	2/64258 (0.0%)
3	SA	0.16	0/1784	0.41	0/2424
4	SB	0.16	0/1765	0.47	0/2362
5	SD	0.17	0/1793	0.44	0/2414
6	SE	0.17	0/2118	0.50	0/2849
7	SF	0.15	0/1481	0.45	0/1988
8	SH	0.22	0/1519	0.62	0/2033
9	SI	0.21	0/1715	0.55	0/2287
10	SK	0.19	0/851	0.45	0/1147
11	SL	0.22	0/1202	0.44	1/1606 (0.1%)
12	SP	0.16	0/1065	0.50	0/1423
13	SQ	0.17	0/1160	0.48	0/1553
14	SR	0.39	0/1105	0.82	4/1484 (0.3%)
15	SS	0.17	0/1216	0.50	0/1628
16	ST	0.16	0/1131	0.41	0/1515
17	SU	0.16	0/831	0.42	0/1115
18	SV	0.14	0/643	0.39	0/860
19	SX	0.15	0/1116	0.42	0/1490
20	Sa	0.16	0/836	0.42	0/1121
21	Sc	0.18	0/508	0.55	2/680 (0.3%)
22	Sd	0.15	0/470	0.58	0/623
23	Sg	0.19	0/2493	0.52	2/3394 (0.1%)
24	SC	0.17	0/1762	0.44	0/2381
25	SG	0.17	0/1946	0.50	0/2590
26	SJ	0.17	0/1550	0.46	0/2069
27	SM	0.21	0/950	0.52	0/1275
28	SN	0.16	0/1232	0.50	1/1656 (0.1%)
29	SO	0.17	0/1023	0.45	0/1372
30	SW	0.17	0/1051	0.50	0/1406
31	SY	0.15	0/1039	0.48	0/1381
32	SZ	0.27	0/604	0.53	0/810

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Sb	0.17	0/665	0.47	0/891
34	Se	0.15	0/465	0.42	0/612
35	Sf	0.18	0/507	0.51	0/673
36	JD	0.15	0/435	0.47	0/581
All	All	0.18	0/81503	0.42	12/118245 (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
7	SF	0	1
13	SQ	0	1
23	Sg	0	1
All	All	0	3

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	SR	109	LEU	CA-C-N	8.77	138.29	121.54
14	SR	109	LEU	C-N-CA	8.77	138.29	121.54
23	Sg	129	ILE	CA-C-N	7.12	135.14	121.54
23	Sg	129	ILE	C-N-CA	7.12	135.14	121.54
2	S2	291	G	C2'-C3'-O3'	6.45	123.37	113.70
21	Sc	34	PHE	CA-C-N	5.55	132.14	121.54
21	Sc	34	PHE	C-N-CA	5.55	132.14	121.54
11	SL	36	TYR	CB-CA-C	-5.43	101.38	110.29
28	SN	134	VAL	N-CA-C	-5.43	107.14	111.81
14	SR	27	ASP	CB-CA-C	-5.35	101.28	110.16
2	S2	112	U	C4'-C3'-O3'	-5.09	105.36	113.00
14	SR	29	HIS	CA-C-O	-5.00	115.23	120.63

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	SF	79	HIS	Peptide
13	SQ	43	GLU	Peptide
23	Sg	129	ILE	Peptide

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	3	0
2	S2	36896	0	18603	387	0
3	SA	1747	0	1751	16	0
4	SB	1738	0	1809	28	0
5	SD	1765	0	1865	18	0
6	SE	2076	0	2177	25	0
7	SF	1461	0	1511	19	0
8	SH	1497	0	1590	18	0
9	SI	1686	0	1772	23	0
10	SK	827	0	854	12	0
11	SL	1182	0	1253	9	0
12	SP	1045	0	1095	16	0
13	SQ	1142	0	1213	24	0
14	SR	1090	0	1149	8	0
15	SS	1198	0	1261	25	0
16	ST	1112	0	1146	15	0
17	SU	821	0	883	8	0
18	SV	636	0	637	9	0
19	SX	1098	0	1167	16	0
20	Sa	821	0	870	8	0
21	Sc	506	0	536	5	0
22	Sd	459	0	451	5	0
23	Sg	2436	0	2393	43	0
24	SC	1725	0	1813	26	0
25	SG	1923	0	2089	34	0
26	SJ	1525	0	1640	22	0
27	SM	940	0	965	14	0
28	SN	1208	0	1294	17	0
29	SO	1010	0	1034	9	0
30	SW	1034	0	1080	16	0
31	SY	1022	0	1088	20	0
32	SZ	598	0	656	12	0
33	Sb	651	0	669	9	0
34	Se	459	0	503	4	0
35	Sf	497	0	496	8	0
36	JD	429	0	415	5	0
37	Sa	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	Sb	1	0	0	0	0
37	Sd	1	0	0	0	0
37	Sf	1	0	0	0	0
All	All	76494	0	60004	798	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 (798) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S2:834:C:N4	2:S2:839:C:H42	1.18	1.35
2:S2:834:C:H42	2:S2:839:C:N4	1.40	1.18
2:S2:24:C:H42	2:S2:650:A:N6	1.46	1.14
2:S2:24:C:N4	2:S2:650:A:H61	1.46	1.11
2:S2:1756:C:N4	2:S2:1775:U:H3	1.51	1.07
2:S2:140:C:N4	2:S2:313:A:H61	1.53	1.06
2:S2:140:C:H42	2:S2:313:A:N6	1.53	1.05
2:S2:533:A:H61	2:S2:550:C:N4	1.58	1.01
2:S2:834:C:N3	2:S2:839:C:N3	2.10	0.98
2:S2:1609:C:N4	2:S2:1630:A:H61	1.63	0.97
2:S2:886:A:N6	2:S2:901:G:C4	2.33	0.97
2:S2:1756:C:H42	2:S2:1775:U:H3	0.96	0.96
2:S2:834:C:N4	2:S2:839:C:N4	2.02	0.95
2:S2:1609:C:H42	2:S2:1630:A:N6	1.64	0.95
2:S2:1271:C:H42	2:S2:1511:U:H3	1.13	0.95
2:S2:694:G:O6	2:S2:737:G:C2	2.21	0.93
2:S2:1533:A:H62	2:S2:1602:U:H3	0.95	0.93
2:S2:1417:C:H42	2:S2:1422:G:N2	1.65	0.92
2:S2:1609:C:H42	2:S2:1630:A:H61	0.94	0.91
2:S2:116:U:H3	2:S2:347:G:H1	1.20	0.90
2:S2:1417:C:H42	2:S2:1422:G:H22	1.10	0.90
2:S2:696:G:H21	2:S2:737:G:H1	1.15	0.89
2:S2:1417:C:N4	2:S2:1422:G:H22	1.70	0.88
2:S2:533:A:N6	2:S2:550:C:H42	1.72	0.86
2:S2:1756:C:N4	2:S2:1775:U:N3	2.24	0.85
2:S2:1652:G:H1	2:S2:1672:U:H3	1.22	0.83
2:S2:1752:C:C4	2:S2:1779:G:N2	2.45	0.83
2:S2:694:G:C6	2:S2:737:G:N2	2.46	0.82
2:S2:1533:A:N6	2:S2:1602:U:H3	1.77	0.81
2:S2:1743:G:H21	2:S2:1791:A:H62	1.28	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S2:748:C:H42	2:S2:795:A:N6	1.78	0.81
33:Sb:37:CYS:HB2	33:Sb:40:CYS:SG	2.22	0.80
2:S2:533:A:N6	2:S2:550:C:N4	2.27	0.79
2:S2:1834:A:N6	2:S2:1836:G:N2	2.30	0.78
2:S2:1287:A:H62	2:S2:1312:G:H21	1.31	0.77
2:S2:810:A:N6	2:S2:851:C:N4	2.32	0.77
2:S2:533:A:H61	2:S2:550:C:H42	1.27	0.76
2:S2:834:C:O2	2:S2:839:C:O2	2.01	0.76
2:S2:563:G:C5	2:S2:586:G:N2	2.54	0.76
2:S2:532:C:C2	2:S2:552:G:N2	2.54	0.76
2:S2:528:A:C2	2:S2:558:G:N1	2.55	0.75
2:S2:528:A:N1	2:S2:558:G:C6	2.54	0.75
2:S2:1:U:C2	2:S2:3:C:N4	2.54	0.75
2:S2:885:U:H3	2:S2:901:G:H1	1.35	0.75
2:S2:1609:C:N3	2:S2:1630:A:N1	2.36	0.74
2:S2:748:C:N4	2:S2:795:A:N6	2.37	0.73
2:S2:528:A:C2	2:S2:558:G:C6	2.77	0.73
2:S2:1615:U:O4	12:SP:40:ARG:NH2	2.22	0.72
2:S2:316:G:H3'	25:SG:183:ARG:HH22	1.55	0.71
2:S2:1756:C:N4	2:S2:1777:G:C6	2.57	0.71
2:S2:878:G:H1	2:S2:908:A:H2	1.38	0.71
2:S2:1076:G:OP2	28:SN:107:LYS:NZ	2.23	0.71
2:S2:748:C:N4	2:S2:795:A:H61	1.89	0.70
2:S2:886:A:N6	2:S2:901:G:C5	2.58	0.70
2:S2:1756:C:N4	2:S2:1777:G:N1	2.38	0.70
2:S2:140:C:N3	2:S2:313:A:N1	2.39	0.70
23:Sg:8:ARG:HH21	23:Sg:311:GLN:HG2	1.57	0.69
2:S2:1417:C:N3	2:S2:1422:G:N1	2.40	0.69
16:ST:85:ASN:HB2	16:ST:88:MET:HB2	1.74	0.69
2:S2:696:G:N2	2:S2:737:G:H1	1.88	0.68
2:S2:694:G:N7	2:S2:696:G:N2	2.42	0.68
2:S2:1017:U:H5'	28:SN:55:ARG:HH11	1.60	0.67
2:S2:532:C:O2	2:S2:552:G:N2	2.27	0.67
10:SK:61:GLN:HB3	10:SK:68:TYR:HB2	1.76	0.67
13:SQ:72:VAL:HG11	13:SQ:80:GLN:HG3	1.77	0.66
2:S2:694:G:O6	2:S2:737:G:N2	2.27	0.66
33:Sb:35:VAL:HG21	33:Sb:63:LEU:HD21	1.78	0.65
9:SI:165:GLN:HE22	9:SI:195:LEU:HD11	1.60	0.65
28:SN:16:LEU:HD12	28:SN:17:PRO:HD2	1.78	0.65
7:SF:124:ASP:OD1	7:SF:125:SER:N	2.29	0.65
2:S2:1488:C:O2'	2:S2:1490:G:OP2	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:SG:49:VAL:HG12	25:SG:115:LYS:HG2	1.79	0.65
19:SX:51:VAL:HG22	19:SX:98:ASP:H	1.62	0.65
2:S2:1752:C:N3	2:S2:1779:G:C2	2.66	0.64
8:SH:66:VAL:HG22	8:SH:96:ALA:HB1	1.79	0.64
3:SA:38:ILE:HD11	3:SA:47:TYR:HB3	1.80	0.64
4:SB:70:SER:OG	29:SO:128:ARG:NH1	2.30	0.64
19:SX:67:ARG:HG3	19:SX:115:ILE:HG12	1.80	0.64
2:S2:878:G:O6	2:S2:908:A:N1	2.30	0.64
2:S2:1756:C:N4	2:S2:1775:U:C4	2.65	0.64
6:SE:63:LYS:HE2	31:SY:85:ASN:HA	1.80	0.63
2:S2:1658:G:OP2	2:S2:1660:C:N4	2.31	0.63
2:S2:1608:U:OP1	15:SS:134:GLN:NE2	2.31	0.62
23:Sg:39:THR:HG22	23:Sg:60:ARG:HG3	1.81	0.62
25:SG:121:ILE:HG22	25:SG:123:GLY:H	1.62	0.62
4:SB:40:ASN:ND2	4:SB:75:GLN:OE1	2.33	0.62
4:SB:47:THR:OG1	4:SB:65:ARG:NH2	2.33	0.62
2:S2:940:U:H3	2:S2:1002:U:H3	1.47	0.62
2:S2:9:U:OP2	36:JD:591:ARG:NH2	2.33	0.61
2:S2:165:G:OP2	2:S2:165:G:N2	2.30	0.61
2:S2:1310:U:OP1	27:SM:36:ARG:NH2	2.33	0.61
4:SB:168:MET:HG2	4:SB:197:ILE:HD13	1.82	0.61
2:S2:925:G:H1	2:S2:1017:U:H3	1.48	0.61
7:SF:74:ASN:OD1	7:SF:86:LYS:NZ	2.33	0.61
24:SC:191:VAL:HG11	24:SC:236:PHE:HA	1.82	0.61
24:SC:196:ILE:HB	24:SC:223:TYR:HB2	1.82	0.61
10:SK:49:MET:HG2	10:SK:52:LEU:HD12	1.82	0.60
10:SK:65:ARG:NH2	22:Sd:21:CYS:O	2.33	0.60
26:SJ:3:VAL:HB	26:SJ:5:ARG:HD3	1.83	0.60
25:SG:147:LEU:HD11	25:SG:151:ASP:HB2	1.83	0.60
2:S2:834:C:H42	2:S2:839:C:H42	0.61	0.60
2:S2:1091:C:HO2'	30:SW:2:VAL:N	1.99	0.60
2:S2:370:G:O2'	9:SI:10:LYS:NZ	2.35	0.60
8:SH:146:VAL:HG22	8:SH:152:ARG:HG2	1.82	0.60
23:Sg:174:VAL:HB	23:Sg:188:HIS:HB2	1.83	0.60
2:S2:165:G:H2'	2:S2:166:A:H8	1.66	0.60
2:S2:436:G:N7	2:S2:471:G:C2	2.70	0.60
32:SZ:99:LEU:HD11	32:SZ:102:LYS:HB2	1.84	0.60
12:SP:111:MET:HE1	15:SS:117:ILE:HA	1.84	0.59
2:S2:874:G:H2'	2:S2:875:A:H8	1.67	0.59
2:S2:880:G:O6	2:S2:906:U:O4	2.20	0.59
12:SP:108:LYS:HB2	12:SP:111:MET:HE3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S2:628:A:OP2	5:SD:179:GLN:NE2	2.34	0.59
31:SY:114:MET:O	31:SY:122:LYS:NZ	2.33	0.59
2:S2:1375:G:H5'	14:SR:67:ARG:HH21	1.67	0.59
11:SL:59:LYS:HD3	11:SL:134:LEU:HB3	1.84	0.59
25:SG:142:ARG:HH21	25:SG:153:VAL:HG11	1.67	0.59
2:S2:1018:U:O2'	28:SN:86:GLU:OE2	2.21	0.59
5:SD:106:ARG:HG3	5:SD:175:VAL:HG22	1.85	0.59
2:S2:919:A:OP2	28:SN:64:ARG:NH2	2.35	0.58
25:SG:7:PHE:HB2	25:SG:124:LEU:HD23	1.84	0.58
25:SG:228:ILE:HG22	25:SG:232:ARG:HH12	1.67	0.58
2:S2:396:U:OP2	11:SL:79:LYS:NZ	2.36	0.58
3:SA:77:ILE:HG21	3:SA:133:PRO:HG2	1.85	0.58
18:SV:16:LYS:NZ	24:SC:257:LYS:O	2.35	0.58
15:SS:46:ARG:NH2	16:ST:50:GLU:OE1	2.36	0.58
15:SS:50:ILE:HD11	15:SS:66:ARG:HH22	1.68	0.58
2:S2:375:U:H4'	11:SL:11:GLN:HE22	1.69	0.58
2:S2:1287:A:H62	2:S2:1312:G:N2	1.99	0.58
23:Sg:87:LEU:HB2	23:Sg:101:PHE:HB2	1.86	0.57
2:S2:1752:C:N3	2:S2:1779:G:N1	2.52	0.57
16:ST:77:LYS:HD2	16:ST:94:ARG:HH21	1.68	0.57
2:S2:532:C:O2	2:S2:552:G:C2	2.58	0.57
23:Sg:191:HIS:ND1	23:Sg:213:ASP:OD2	2.33	0.57
2:S2:1:U:C2	2:S2:3:C:C4	2.92	0.57
2:S2:1299:A:OP1	12:SP:59:ARG:NH1	2.38	0.57
24:SC:66:LEU:HD13	24:SC:86:LEU:HD22	1.87	0.57
6:SE:59:ASP:OD1	6:SE:62:LYS:NZ	2.37	0.57
11:SL:90:ARG:HD2	11:SL:109:MET:HE2	1.85	0.57
2:S2:810:A:C6	2:S2:851:C:C4	2.93	0.57
2:S2:844:U:H2'	2:S2:845:G:H8	1.69	0.57
2:S2:886:A:C6	2:S2:901:G:C4	2.93	0.57
17:SU:80:PHE:HB3	22:Sd:52:PHE:HB3	1.87	0.57
23:Sg:165:ILE:HG23	23:Sg:177:TRP:HB2	1.86	0.57
2:S2:1647:A:OP1	13:SQ:138:ARG:NH2	2.38	0.56
7:SF:127:ARG:HB3	7:SF:136:ARG:HB2	1.88	0.56
2:S2:659:G:H21	19:SX:17:ARG:HH22	1.53	0.56
4:SB:149:GLN:NE2	4:SB:151:ARG:O	2.37	0.56
27:SM:20:GLU:HA	27:SM:23:LYS:HG2	1.87	0.56
5:SD:211:VAL:HG21	36:JD:640:ARG:HH21	1.70	0.56
19:SX:134:TYR:O	34:Se:13:ARG:NH2	2.39	0.56
24:SC:252:THR:HG22	24:SC:254:ASP:H	1.71	0.56
2:S2:906:U:H2'	2:S2:907:G:H8	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:SH:143:ARG:HB2	8:SH:155:LYS:HB2	1.85	0.56
11:SL:38:LYS:NZ	11:SL:64:GLY:O	2.36	0.56
28:SN:99:ARG:NH2	28:SN:119:GLU:OE2	2.39	0.56
2:S2:24:C:N3	2:S2:650:A:N1	2.53	0.56
2:S2:69:C:OP2	25:SG:167:LYS:NZ	2.36	0.56
2:S2:326:C:O2	2:S2:327:G:N2	2.39	0.56
2:S2:1016:U:H5''	28:SN:14:SER:HB3	1.87	0.56
2:S2:1259:A:N6	2:S2:1519:U:OP1	2.36	0.56
28:SN:46:THR:OG1	28:SN:86:GLU:OE1	2.23	0.56
2:S2:65:C:N4	25:SG:134:GLY:O	2.38	0.56
2:S2:1617:G:N1	2:S2:1620:A:OP2	2.39	0.56
2:S2:1679:A:H2'	7:SF:60:ARG:HD2	1.86	0.56
2:S2:1752:C:C2	2:S2:1779:G:N1	2.74	0.56
2:S2:1244:U:H2'	2:S2:1245:G:H8	1.70	0.55
2:S2:1551:U:OP1	5:SD:9:ARG:NH2	2.39	0.55
18:SV:80:SER:OG	18:SV:82:ASN:OD1	2.25	0.55
6:SE:88:ASP:OD1	6:SE:122:LYS:NZ	2.32	0.55
23:Sg:66:VAL:HA	23:Sg:82:SER:HA	1.87	0.55
25:SG:84:TYR:HE2	25:SG:93:LYS:HB3	1.71	0.55
2:S2:697:G:OP2	2:S2:733:C:N4	2.40	0.55
2:S2:1290:G:O6	35:Sf:95:ARG:NH2	2.40	0.55
7:SF:89:THR:HA	7:SF:92:ILE:HG12	1.89	0.55
31:SY:4:THR:OG1	31:SY:32:LYS:NZ	2.39	0.55
2:S2:49:C:H2'	2:S2:472:C:H41	1.71	0.55
2:S2:643:A:OP1	26:SJ:38:ARG:NH1	2.39	0.55
2:S2:1010:G:H2'	2:S2:1011:A:H8	1.72	0.55
4:SB:88:THR:HA	4:SB:98:THR:HA	1.88	0.55
2:S2:1854:U:H2'	2:S2:1855:G:H8	1.72	0.55
2:S2:377:G:H5'	9:SI:98:LYS:HB3	1.87	0.55
2:S2:1417:C:O2	2:S2:1422:G:O6	2.25	0.55
16:ST:129:ARG:HH11	16:ST:133:ARG:HH21	1.55	0.55
2:S2:747:U:N3	2:S2:796:G:N1	2.55	0.55
2:S2:886:A:C5	2:S2:901:G:C2	2.95	0.55
2:S2:921:G:O6	30:SW:60:LYS:NZ	2.40	0.55
23:Sg:62:HIS:NE2	23:Sg:80:SER:OG	2.36	0.55
2:S2:1228:A:H2'	2:S2:1229:G:C8	2.42	0.54
29:SO:62:VAL:HG21	29:SO:67:ASP:HB2	1.89	0.54
2:S2:1122:A:N3	4:SB:146:ARG:NH1	2.54	0.54
23:Sg:26:GLN:NE2	23:Sg:73:SER:O	2.39	0.54
6:SE:212:ASP:OD1	6:SE:213:ALA:N	2.40	0.54
23:Sg:17:TRP:HB2	23:Sg:36:ARG:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:SJ:82:VAL:HG21	26:SJ:92:MET:HE1	1.90	0.54
2:S2:913:A:H1'	8:SH:66:VAL:HB	1.89	0.54
8:SH:69:LEU:HD12	8:SH:96:ALA:HB2	1.90	0.54
2:S2:1542:C:OP1	16:ST:62:ARG:NH1	2.40	0.54
5:SD:137:VAL:HG22	5:SD:151:LYS:HG3	1.89	0.54
9:SI:98:LYS:HG3	9:SI:178:ARG:HG2	1.90	0.54
2:S2:928:G:H2'	2:S2:929:G:C8	2.43	0.54
13:SQ:50:LYS:HA	13:SQ:53:GLU:HG3	1.90	0.54
27:SM:85:LEU:HA	27:SM:88:TRP:HB2	1.88	0.54
2:S2:1834:A:C5	2:S2:1836:G:C2	2.96	0.54
23:Sg:123:GLY:HA2	23:Sg:129:ILE:HG23	1.89	0.54
2:S2:126:G:OP2	25:SG:198:ARG:NH2	2.40	0.54
13:SQ:130:LYS:NZ	13:SQ:134:GLY:O	2.40	0.54
23:Sg:110:SER:O	23:Sg:123:GLY:N	2.35	0.54
28:SN:67:THR:OG1	28:SN:68:GLY:N	2.35	0.54
2:S2:380:G:OP1	9:SI:56:ARG:NH2	2.41	0.54
2:S2:1354:G:N2	2:S2:1357:A:OP2	2.34	0.54
4:SB:70:SER:HA	4:SB:83:LYS:HA	1.90	0.54
6:SE:127:ARG:HH21	6:SE:142:HIS:HB2	1.73	0.54
11:SL:151:THR:OG1	11:SL:152:LYS:N	2.41	0.54
2:S2:5:U:H2'	2:S2:6:G:H8	1.72	0.53
4:SB:34:LYS:NZ	4:SB:43:ASN:OD1	2.36	0.53
13:SQ:127:CYS:SG	13:SQ:128:GLU:N	2.82	0.53
2:S2:56:G:OP1	31:SY:111:LYS:NZ	2.40	0.53
2:S2:1743:G:N2	2:S2:1791:A:H62	1.99	0.53
13:SQ:32:ILE:HG22	13:SQ:68:ILE:HB	1.89	0.53
13:SQ:53:GLU:OE1	13:SQ:85:ARG:NH2	2.39	0.53
2:S2:687:C:OP1	30:SW:32:LYS:NZ	2.41	0.53
27:SM:42:LEU:HD13	27:SM:68:LEU:HB3	1.89	0.53
18:SV:1:MET:HA	18:SV:9:VAL:HG12	1.90	0.53
2:S2:1209:A:O2'	20:Sa:85:ARG:NH1	2.40	0.53
13:SQ:19:ALA:HB2	13:SQ:75:GLY:HA3	1.90	0.53
27:SM:49:LEU:HD11	27:SM:77:ILE:HG12	1.91	0.53
35:Sf:99:LYS:HD3	35:Sf:100:LEU:HD23	1.89	0.53
26:SJ:46:VAL:HG13	26:SJ:102:ILE:HD11	1.90	0.53
31:SY:44:LEU:HD23	31:SY:75:ILE:HD11	1.90	0.53
2:S2:94:G:O2'	2:S2:508:A:O2'	2.27	0.53
6:SE:73:ASP:OD2	6:SE:122:LYS:NZ	2.40	0.53
6:SE:247:THR:OG1	6:SE:250:GLU:OE1	2.25	0.53
7:SF:71:ARG:NH2	7:SF:148:ASN:OD1	2.42	0.53
23:Sg:46:THR:HG23	23:Sg:53:GLY:HA2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:SG:22:ARG:HH12	25:SG:25:ARG:HD3	1.73	0.53
2:S2:146:G:H1	2:S2:173:A:H61	1.55	0.53
2:S2:974:C:H2'	2:S2:975:G:H8	1.74	0.53
2:S2:1004:U:H2'	2:S2:1005:G:H8	1.74	0.53
19:SX:140:ARG:HD2	19:SX:141:PRO:HD2	1.91	0.53
32:SZ:58:LEU:HD12	32:SZ:62:VAL:HG21	1.90	0.53
2:S2:1144:A:H5'	2:S2:1355:C:H41	1.74	0.53
2:S2:1396:A:O2'	2:S2:1398:G:N7	2.41	0.53
12:SP:50:ARG:N	12:SP:53:GLN:OE1	2.42	0.53
31:SY:100:LYS:NZ	31:SY:101:LYS:O	2.41	0.53
23:Sg:5:MET:HB2	23:Sg:270:LEU:HD21	1.90	0.52
14:SR:57:LEU:HA	14:SR:60:ARG:HG3	1.90	0.52
23:Sg:110:SER:HB2	23:Sg:155:ARG:HH12	1.74	0.52
2:S2:886:A:C6	2:S2:901:G:N3	2.77	0.52
2:S2:1130:G:OP2	2:S2:1130:G:N2	2.36	0.52
2:S2:1566:G:N7	16:ST:101:ARG:NH2	2.57	0.52
24:SC:187:ARG:HE	24:SC:192:LEU:HD12	1.74	0.52
2:S2:71:G:N7	25:SG:170:ARG:NH2	2.55	0.52
2:S2:528:A:N1	2:S2:558:G:O6	2.42	0.52
2:S2:695:C:N4	2:S2:736:C:O2'	2.43	0.52
2:S2:1388:A:H61	5:SD:161:GLY:HA3	1.75	0.52
7:SF:49:LEU:HD12	13:SQ:50:LYS:HG3	1.90	0.52
23:Sg:14:HIS:NE2	23:Sg:33:SER:OG	2.38	0.52
23:Sg:40:ILE:HD11	23:Sg:66:VAL:HG21	1.90	0.52
27:SM:54:SER:HB3	27:SM:78:LYS:HD2	1.91	0.52
2:S2:190:G:OP1	9:SI:149:TYR:OH	2.25	0.52
2:S2:4:C:H4'	24:SC:207:ALA:HB2	1.91	0.52
2:S2:122:G:OP1	6:SE:75:LYS:NZ	2.43	0.52
8:SH:144:ILE:HB	30:SW:52:ILE:HB	1.92	0.52
2:S2:113:G:C8	2:S2:113:G:H5'	2.45	0.52
2:S2:613:G:N2	2:S2:626:G:OP1	2.41	0.52
2:S2:810:A:N6	2:S2:851:C:C4	2.78	0.52
2:S2:483:C:H5''	19:SX:48:LYS:HE3	1.91	0.52
7:SF:28:VAL:O	7:SF:42:LYS:NZ	2.37	0.52
8:SH:78:ARG:HG2	8:SH:81:ARG:HH21	1.74	0.52
6:SE:95:THR:HG22	31:SY:16:ARG:HB2	1.92	0.52
2:S2:1310:U:H4'	35:Sf:143:LYS:HG3	1.92	0.51
2:S2:420:G:O2'	2:S2:660:C:N3	2.41	0.51
2:S2:1228:A:H2'	2:S2:1229:G:H8	1.75	0.51
2:S2:846:G:OP1	6:SE:106:LYS:NZ	2.41	0.51
8:SH:100:ILE:HG12	8:SH:125:VAL:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:SQ:8:GLN:HG2	13:SQ:99:TYR:HE2	1.76	0.51
15:SS:137:LYS:HG2	15:SS:138:THR:HG23	1.91	0.51
25:SG:63:MET:HE3	25:SG:100:CYS:HA	1.91	0.51
2:S2:1171:G:O2'	2:S2:1187:G:O6	2.26	0.51
2:S2:1752:C:H42	2:S2:1778:C:H42	1.59	0.51
2:S2:1808:U:H2'	2:S2:1809:A:H8	1.75	0.51
4:SB:167:LYS:HA	4:SB:170:GLU:HG2	1.93	0.51
2:S2:1550:G:O2'	2:S2:1558:C:O2	2.28	0.51
7:SF:50:PRO:HB3	7:SF:69:VAL:HG13	1.92	0.51
23:Sg:47:ARG:HE	23:Sg:52:TYR:HE1	1.57	0.51
2:S2:857:U:H2'	2:S2:858:A:C8	2.46	0.51
2:S2:1533:A:N6	2:S2:1602:U:C2	2.79	0.51
7:SF:103:LEU:O	32:SZ:66:LYS:NZ	2.39	0.51
2:S2:604:A:N3	2:S2:639:C:O2'	2.37	0.51
2:S2:1752:C:C4	2:S2:1779:G:C2	2.98	0.51
25:SG:32:MET:HA	25:SG:52:ILE:HG23	1.93	0.51
25:SG:98:ARG:NH2	25:SG:105:ASN:O	2.43	0.51
27:SM:46:GLN:HE21	27:SM:112:LYS:HD3	1.75	0.51
4:SB:36:PRO:HB3	4:SB:231:LEU:HG	1.92	0.51
6:SE:60:GLU:OE1	31:SY:20:ARG:NH2	2.33	0.51
8:SH:127:ASP:OD1	8:SH:142:LYS:NZ	2.43	0.51
2:S2:466:G:O2'	2:S2:467:G:O4'	2.21	0.51
8:SH:10:LYS:HZ1	8:SH:14:GLU:H	1.59	0.51
2:S2:563:G:C6	2:S2:586:G:N2	2.79	0.50
2:S2:1613:G:OP2	12:SP:39:ALA:N	2.44	0.50
23:Sg:11:LEU:HB2	23:Sg:307:VAL:HB	1.93	0.50
1:Ln:11:ARG:NH1	2:S2:1845:A:OP2	2.45	0.50
4:SB:97:LEU:HB3	4:SB:232:HIS:CE1	2.46	0.50
31:SY:78:SER:OG	31:SY:80:ASP:OD1	2.29	0.50
2:S2:1834:A:C6	2:S2:1836:G:N2	2.79	0.50
4:SB:138:PHE:O	4:SB:213:ARG:N	2.42	0.50
2:S2:1288:U:O4	2:S2:1311:C:N3	2.45	0.50
28:SN:5:HIS:HB3	28:SN:117:LEU:HD23	1.94	0.50
2:S2:560:A:O5'	26:SJ:174:LYS:NZ	2.43	0.50
13:SQ:97:GLN:HB2	13:SQ:105:LYS:HG3	1.93	0.50
15:SS:15:VAL:HB	15:SS:20:ILE:HG13	1.94	0.50
16:ST:28:LEU:HD13	16:ST:110:LEU:HD22	1.92	0.50
17:SU:51:LYS:HB3	17:SU:90:ASP:HB2	1.94	0.50
23:Sg:23:THR:HG21	23:Sg:292:SER:HA	1.94	0.50
23:Sg:57:ARG:HD3	23:Sg:95:GLY:HA3	1.92	0.50
25:SG:33:ALA:HA	25:SG:51:ARG:HD3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:SG:67:VAL:HG12	25:SG:69:THR:HG22	1.93	0.50
2:S2:1:U:O2	2:S2:3:C:C4	2.65	0.49
2:S2:168:C:O2'	25:SG:133:LEU:O	2.29	0.49
2:S2:1143:A:H5'	24:SC:190:SER:HB3	1.94	0.49
30:SW:17:ALA:HB1	30:SW:22:LYS:HG3	1.93	0.49
2:S2:145:G:H2'	2:S2:146:G:C8	2.47	0.49
5:SD:227:LYS:N	23:Sg:185:LYS:O	2.41	0.49
17:SU:55:ARG:HH11	17:SU:87:ARG:HE	1.59	0.49
2:S2:1287:A:N6	2:S2:1312:G:H21	2.05	0.49
18:SV:14:PRO:HG3	24:SC:248:TYR:CZ	2.46	0.49
26:SJ:170:PRO:O	26:SJ:175:ARG:NH1	2.44	0.49
2:S2:1597:C:OP2	32:SZ:85:ARG:NH2	2.46	0.49
2:S2:671:A:H4'	2:S2:672:A:H5''	1.94	0.49
4:SB:71:LEU:HD11	4:SB:189:ILE:HG23	1.94	0.49
6:SE:160:ILE:HD12	6:SE:169:ILE:HG12	1.94	0.49
2:S2:28:U:H2'	2:S2:29:G:H8	1.77	0.49
2:S2:436:G:C8	2:S2:471:G:C2	3.00	0.49
4:SB:33:VAL:HG12	4:SB:96:CYS:HB2	1.95	0.49
2:S2:846:G:C4	6:SE:19:MET:HE2	2.47	0.49
5:SD:207:HIS:CD2	36:JD:634:LYS:HA	2.48	0.49
21:Sc:21:THR:HB	21:Sc:68:LEU:HD11	1.93	0.49
23:Sg:130:LYS:HG2	23:Sg:141:THR:HG23	1.94	0.49
2:S2:351:G:OP1	9:SI:7:ASN:ND2	2.32	0.49
23:Sg:31:ILE:HG12	23:Sg:45:LEU:HD11	1.95	0.49
24:SC:271:ASP:OD1	24:SC:271:ASP:N	2.46	0.49
2:S2:106:C:H2'	2:S2:107:A:H8	1.78	0.49
2:S2:186:C:H2'	2:S2:187:G:H8	1.77	0.49
12:SP:81:ARG:HH12	12:SP:120:SER:HB3	1.78	0.49
25:SG:1:MET:HE3	25:SG:24:LEU:HD22	1.94	0.49
26:SJ:127:ARG:HD3	34:Se:31:ARG:HD3	1.93	0.49
29:SO:101:GLY:HA3	29:SO:134:PRO:HD2	1.94	0.49
2:S2:1047:C:H5'	29:SO:143:LYS:HB2	1.95	0.48
2:S2:1155:U:OP1	24:SC:185:THR:OG1	2.28	0.48
21:Sc:13:ARG:HB2	21:Sc:55:VAL:HG12	1.95	0.48
23:Sg:144:ASP:OD1	23:Sg:144:ASP:N	2.46	0.48
32:SZ:69:THR:HG22	32:SZ:72:VAL:HG22	1.95	0.48
2:S2:1677:U:H2'	2:S2:1678:A:H8	1.78	0.48
29:SO:98:ARG:HB3	29:SO:132:VAL:HG23	1.94	0.48
2:S2:1467:C:OP1	14:SR:1:MET:N	2.46	0.48
4:SB:44:ILE:HG23	4:SB:69:VAL:HG21	1.95	0.48
16:ST:40:ALA:HB3	16:ST:43:LYS:HG2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S2:5:U:H2'	2:S2:6:G:C8	2.49	0.48
2:S2:455:A:H2'	2:S2:456:C:C6	2.48	0.48
20:Sa:11:ALA:HB3	20:Sa:33:ASP:HB2	1.95	0.48
2:S2:649:U:H2'	2:S2:650:A:H8	1.77	0.48
15:SS:24:ARG:HB2	15:SS:29:ALA:HB2	1.95	0.48
24:SC:184:VAL:HG11	24:SC:247:THR:HG22	1.94	0.48
30:SW:104:LEU:HD23	30:SW:125:ILE:HA	1.95	0.48
3:SA:190:SER:OG	3:SA:192:GLU:OE1	2.32	0.48
7:SF:34:SER:OG	7:SF:146:ARG:NH2	2.40	0.48
7:SF:34:SER:HA	21:Sc:55:VAL:HG23	1.95	0.48
19:SX:104:GLY:HA2	19:SX:120:PHE:HD1	1.78	0.48
24:SC:172:ASN:ND2	26:SJ:95:ASP:OD2	2.44	0.48
24:SC:183:LYS:HE3	24:SC:196:ILE:HD12	1.95	0.48
2:S2:617:G:C6	2:S2:625:G:C2	3.02	0.48
9:SI:57:ALA:HB2	9:SI:183:GLY:HA2	1.95	0.48
26:SJ:111:GLN:NE2	26:SJ:127:ARG:HB2	2.29	0.48
31:SY:12:PHE:HE1	31:SY:21:LYS:HB3	1.78	0.48
2:S2:158:A:C2	2:S2:463:C:O2	2.67	0.48
2:S2:959:G:OP1	29:SO:104:ARG:NH2	2.46	0.48
26:SJ:22:LYS:NZ	26:SJ:26:ASP:OD2	2.46	0.48
2:S2:77:A:O2'	25:SG:174:PRO:O	2.29	0.48
12:SP:96:VAL:O	12:SP:103:ASN:N	2.47	0.48
2:S2:1834:A:C6	2:S2:1836:G:C2	3.01	0.48
30:SW:11:LEU:HD12	30:SW:72:CYS:HB2	1.96	0.48
3:SA:118:GLU:HB2	24:SC:65:LYS:NZ	2.28	0.47
6:SE:18:TRP:HH2	6:SE:31:PRO:HD3	1.78	0.47
8:SH:10:LYS:HZ1	8:SH:14:GLU:HB2	1.78	0.47
8:SH:68:GLN:O	8:SH:71:SER:OG	2.28	0.47
1:Ln:12:ARG:NH2	2:S2:1847:G:N7	2.62	0.47
27:SM:20:GLU:HG2	27:SM:119:GLN:HB2	1.96	0.47
1:Ln:1:MET:HE3	2:S2:1851:A:H5''	1.96	0.47
2:S2:436:G:C8	2:S2:471:G:N2	2.82	0.47
18:SV:25:GLY:O	24:SC:85:SER:OG	2.33	0.47
27:SM:24:THR:HA	27:SM:27:ILE:HG12	1.97	0.47
28:SN:55:ARG:NH2	33:Sb:51:GLN:OE1	2.47	0.47
2:S2:391:C:H2'	2:S2:392:A:H8	1.80	0.47
2:S2:508:A:H3'	2:S2:509:G:H8	1.78	0.47
2:S2:1541:G:H4'	16:ST:15:VAL:HG11	1.96	0.47
15:SS:89:ASP:OD1	15:SS:90:VAL:N	2.48	0.47
17:SU:35:VAL:HG21	17:SU:110:VAL:HG11	1.96	0.47
2:S2:616:A:H62	2:S2:625:G:H21	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S2:969:U:O2	2:S2:971:G:N1	2.47	0.47
2:S2:1389:C:O2'	5:SD:162:ASP:OD1	2.27	0.47
2:S2:1653:U:H3	2:S2:1671:G:H1	1.61	0.47
2:S2:1764:G:H5'	2:S2:1765:C:H5''	1.96	0.47
25:SG:98:ARG:HE	25:SG:106:LEU:HD13	1.80	0.47
2:S2:694:G:N7	2:S2:696:G:C2	2.83	0.47
7:SF:38:TYR:HE2	7:SF:143:PRO:HB2	1.80	0.47
26:SJ:46:VAL:HG11	26:SJ:106:LEU:HD21	1.97	0.47
2:S2:67:C:OP1	25:SG:160:LYS:NZ	2.38	0.47
2:S2:528:A:C2	2:S2:558:G:C2	3.03	0.47
2:S2:808:A:H2	2:S2:855:G:H22	1.63	0.47
2:S2:888:U:H2'	2:S2:900:C:H42	1.79	0.47
2:S2:1035:A:O2'	2:S2:1856:C:O2	2.32	0.47
2:S2:1650:A:H5''	13:SQ:139:ALA:HB2	1.97	0.47
16:ST:76:THR:HG23	16:ST:94:ARG:HD3	1.95	0.47
2:S2:106:C:H2'	2:S2:107:A:C8	2.50	0.47
2:S2:691:G:N2	2:S2:691:G:OP2	2.48	0.47
2:S2:880:G:O6	2:S2:906:U:C4	2.68	0.47
26:SJ:63:LEU:HD11	26:SJ:69:ARG:HH21	1.80	0.47
2:S2:563:G:H1	2:S2:592:C:H5	1.61	0.46
2:S2:1513:C:H2'	2:S2:1514:G:H8	1.79	0.46
17:SU:55:ARG:NH1	17:SU:87:ARG:HE	2.14	0.46
24:SC:214:LEU:HD23	24:SC:244:ILE:HD11	1.96	0.46
2:S2:329:G:H2'	2:S2:330:G:C8	2.51	0.46
3:SA:118:GLU:HB2	24:SC:65:LYS:HZ1	1.80	0.46
15:SS:115:LYS:HD3	15:SS:126:PHE:HB2	1.97	0.46
24:SC:106:VAL:HG22	24:SC:128:VAL:HG22	1.98	0.46
29:SO:54:CYS:HB3	29:SO:81:VAL:HG23	1.96	0.46
2:S2:1086:G:OP2	20:Sa:12:LYS:NZ	2.42	0.46
24:SC:116:THR:HG21	24:SC:121:ARG:HH21	1.81	0.46
2:S2:107:A:H2'	2:S2:108:G:C8	2.50	0.46
2:S2:550:C:H2'	2:S2:551:U:C6	2.51	0.46
2:S2:1098:C:H2'	2:S2:1099:G:C8	2.50	0.46
2:S2:1832:A:H5''	2:S2:1840:U:H5''	1.97	0.46
3:SA:10:MET:HE1	3:SA:51:LEU:HB3	1.96	0.46
10:SK:25:LYS:HA	10:SK:46:MET:HE1	1.98	0.46
3:SA:33:GLN:HB2	3:SA:154:LEU:HD13	1.96	0.46
6:SE:21:ASP:OD1	6:SE:23:LEU:N	2.46	0.46
20:Sa:87:ARG:NH1	20:Sa:91:ALA:O	2.48	0.46
30:SW:27:ILE:HB	30:SW:61:ILE:HB	1.98	0.46
31:SY:76:TYR:OH	31:SY:85:ASN:O	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S2:477:G:H2'	2:S2:478:G:C8	2.50	0.46
2:S2:902:G:O2'	2:S2:903:A:O4'	2.33	0.46
2:S2:1610:G:O2'	15:SS:86:ARG:NH2	2.44	0.46
25:SG:181:THR:HG23	25:SG:184:VAL:H	1.81	0.46
2:S2:1220:A:N3	2:S2:1677:U:O2'	2.41	0.46
2:S2:1403:C:N4	2:S2:1433:C:OP1	2.49	0.46
2:S2:1779:G:H2'	2:S2:1780:G:C8	2.51	0.46
2:S2:600:G:H2'	2:S2:601:G:H8	1.80	0.45
6:SE:204:SER:OG	6:SE:205:PHE:N	2.47	0.45
22:Sd:6:LEU:HA	22:Sd:9:SER:HB3	1.99	0.45
24:SC:194:ARG:HD3	24:SC:196:ILE:HD11	1.97	0.45
26:SJ:108:ARG:HH22	26:SJ:154:GLN:HG3	1.80	0.45
26:SJ:142:VAL:HG12	26:SJ:144:ILE:H	1.81	0.45
2:S2:886:A:N7	2:S2:901:G:C2	2.83	0.45
2:S2:943:U:OP1	4:SB:214:LYS:NZ	2.49	0.45
2:S2:1203:G:H4'	24:SC:116:THR:HA	1.98	0.45
14:SR:71:ILE:HG22	14:SR:74:GLN:H	1.80	0.45
17:SU:22:ILE:HB	17:SU:89:ILE:HB	1.98	0.45
2:S2:158:A:H2	2:S2:463:C:H1'	1.80	0.45
2:S2:570:C:O2'	31:SY:34:THR:O	2.31	0.45
2:S2:1128:C:H2'	2:S2:1129:G:C8	2.50	0.45
12:SP:22:LEU:HA	12:SP:25:LEU:HD12	1.98	0.45
12:SP:64:LYS:NZ	12:SP:88:GLU:O	2.47	0.45
13:SQ:47:LEU:HD23	13:SQ:50:LYS:HD3	1.97	0.45
13:SQ:90:LYS:HE2	13:SQ:90:LYS:HB3	1.70	0.45
32:SZ:102:LYS:HA	32:SZ:107:VAL:HG23	1.98	0.45
2:S2:671:A:OP1	2:S2:1163:C:O2'	2.32	0.45
10:SK:58:VAL:HG12	10:SK:71:LEU:HA	1.98	0.45
12:SP:92:SER:H	12:SP:107:ILE:HB	1.81	0.45
2:S2:528:A:N1	2:S2:529:A:N6	2.65	0.45
2:S2:934:G:H22	2:S2:1008:A:H2	1.63	0.45
2:S2:1083:A:N7	2:S2:1841:C:O2'	2.39	0.45
2:S2:1656:G:H1	2:S2:1668:U:H3	1.64	0.45
22:Sd:26:ASN:OD1	22:Sd:27:ARG:N	2.49	0.45
25:SG:48:TYR:HE1	25:SG:117:GLY:H	1.63	0.45
2:S2:750:C:H41	2:S2:793:G:H21	1.64	0.45
24:SC:110:MET:HG3	24:SC:125:LYS:HB3	1.98	0.45
31:SY:11:LYS:HB2	31:SY:24:VAL:HG12	1.99	0.45
2:S2:640:A:H2'	2:S2:641:A:C8	2.51	0.45
2:S2:1726:G:H1	2:S2:1808:U:H3	1.63	0.45
8:SH:144:ILE:N	30:SW:51:GLU:OE2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:SX:46:HIS:CD2	19:SX:103:ALA:HB2	2.52	0.45
23:Sg:126:ASP:OD1	23:Sg:126:ASP:N	2.49	0.45
23:Sg:274:VAL:HG22	23:Sg:277:THR:HG22	1.99	0.45
25:SG:50:VAL:HG23	25:SG:113:ILE:HD13	1.97	0.45
2:S2:962:A:N1	2:S2:1055:A:O2'	2.50	0.45
4:SB:126:ASP:OD1	4:SB:136:ARG:NE	2.50	0.45
15:SS:5:ILE:HA	32:SZ:49:LEU:HD23	1.99	0.45
16:ST:114:GLU:OE1	16:ST:114:GLU:N	2.50	0.45
19:SX:68:LYS:HB3	19:SX:91:LEU:HD22	1.99	0.45
33:Sb:36:LYS:NZ	33:Sb:40:CYS:O	2.44	0.45
35:Sf:118:ARG:HB2	35:Sf:131:PHE:HD2	1.82	0.45
6:SE:11:ARG:HA	6:SE:28:ALA:HB2	1.98	0.45
19:SX:125:VAL:HG22	19:SX:140:ARG:HH12	1.82	0.45
7:SF:179:ASN:HB2	7:SF:187:SER:HB2	1.99	0.45
9:SI:56:ARG:HA	9:SI:56:ARG:HD3	1.72	0.45
31:SY:76:TYR:OH	31:SY:86:GLU:OE1	2.30	0.45
2:S2:1144:A:H2'	2:S2:1145:A:C8	2.52	0.44
2:S2:1221:G:H2'	2:S2:1222:G:C8	2.52	0.44
3:SA:115:ALA:HB1	3:SA:117:ARG:HH22	1.82	0.44
13:SQ:15:ARG:O	13:SQ:86:GLN:NE2	2.51	0.44
15:SS:22:GLY:HA2	15:SS:56:ALA:HB3	1.98	0.44
18:SV:16:LYS:HE2	24:SC:259:THR:HG23	1.99	0.44
26:SJ:136:ARG:HA	26:SJ:141:VAL:HA	1.98	0.44
2:S2:1373:C:OP1	14:SR:7:LYS:N	2.50	0.44
3:SA:37:TYR:OH	3:SA:57:LYS:NZ	2.40	0.44
3:SA:198:MET:HG3	3:SA:200:ASP:H	1.82	0.44
13:SQ:102:GLU:HA	13:SQ:105:LYS:HB3	1.99	0.44
15:SS:88:LYS:H	15:SS:95:TYR:HD1	1.65	0.44
2:S2:1277:C:H2'	2:S2:1278:A:H8	1.83	0.44
2:S2:1736:G:H2'	2:S2:1737:G:C8	2.52	0.44
4:SB:99:ASN:OD1	4:SB:100:PHE:N	2.50	0.44
23:Sg:245:ARG:HD2	23:Sg:247:TRP:CE2	2.51	0.44
2:S2:1017:U:OP2	28:SN:55:ARG:NH1	2.50	0.44
2:S2:1034:A:H61	2:S2:1843:G:H1'	1.81	0.44
2:S2:839:C:O2'	2:S2:841:G:O4'	2.36	0.44
2:S2:943:U:H2'	2:S2:944:A:C8	2.52	0.44
2:S2:1129:G:H5''	33:Sb:22:LYS:HE3	1.98	0.44
12:SP:86:LEU:H	12:SP:89:MET:HE3	1.82	0.44
15:SS:31:THR:HA	15:SS:36:VAL:HG13	1.98	0.44
2:S2:566:U:H3	2:S2:584:G:H1	1.66	0.44
2:S2:639:C:OP1	34:Se:41:ARG:NH2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S2:1350:U:H1'	3:SA:112:ILE:HD11	1.99	0.44
6:SE:36:HIS:CE1	6:SE:85:GLY:HA3	2.53	0.44
7:SF:79:HIS:O	7:SF:81:ARG:N	2.51	0.44
32:SZ:84:ALA:O	32:SZ:88:LEU:HD13	2.18	0.44
2:S2:345:U:OP1	6:SE:37:LYS:NZ	2.42	0.44
2:S2:1221:G:H2'	2:S2:1222:G:H8	1.83	0.44
27:SM:29:ASP:OD1	27:SM:30:GLY:N	2.50	0.44
2:S2:931:C:H2'	2:S2:932:G:C8	2.53	0.44
2:S2:1004:U:H2'	2:S2:1005:G:C8	2.53	0.44
3:SA:31:ASP:OD1	3:SA:32:PHE:N	2.51	0.44
10:SK:95:ARG:HH22	10:SK:98:ARG:HA	1.83	0.44
13:SQ:50:LYS:HB3	13:SQ:50:LYS:HE3	1.74	0.44
18:SV:39:VAL:HB	18:SV:44:GLY:HA2	1.98	0.44
35:Sf:123:SER:HB2	35:Sf:126:CYS:HB2	1.99	0.44
2:S2:1010:G:H2'	2:S2:1011:A:C8	2.52	0.44
5:SD:225:GLU:HB2	23:Sg:187:ASN:HB3	2.00	0.44
30:SW:11:LEU:HD11	30:SW:37:PHE:HE2	1.83	0.44
2:S2:979:C:H2'	2:S2:980:A:H8	1.82	0.43
2:S2:1232:U:H2'	2:S2:1233:G:H8	1.82	0.43
9:SI:78:ILE:HD13	9:SI:96:LEU:HD11	1.99	0.43
12:SP:37:TYR:OH	12:SP:85:ILE:O	2.32	0.43
14:SR:28:PHE:HA	14:SR:55:THR:HG21	2.00	0.43
2:S2:153:G:H2'	2:S2:154:U:C6	2.54	0.43
2:S2:979:C:H2'	2:S2:980:A:C8	2.53	0.43
2:S2:1539:U:H4'	16:ST:47:PRO:HA	2.00	0.43
2:S2:1610:G:HO2'	15:SS:86:ARG:NH2	2.16	0.43
5:SD:136:VAL:HG22	5:SD:186:VAL:HG22	1.99	0.43
10:SK:14:LEU:HD22	10:SK:35:LEU:HD11	2.00	0.43
23:Sg:173:LEU:HD23	23:Sg:187:ASN:HD21	1.83	0.43
27:SM:68:LEU:HD22	35:Sf:114:ILE:HG13	2.00	0.43
2:S2:395:G:N2	9:SI:14:THR:O	2.43	0.43
2:S2:693:A:C2	2:S2:694:G:O6	2.72	0.43
2:S2:1653:U:H2'	2:S2:1654:G:C8	2.54	0.43
9:SI:6:ASP:OD1	9:SI:9:HIS:ND1	2.48	0.43
17:SU:19:ARG:HH11	17:SU:92:HIS:HB3	1.83	0.43
18:SV:60:ARG:HA	18:SV:65:SER:HB2	1.99	0.43
26:SJ:110:LEU:HB2	26:SJ:147:PHE:HB3	2.00	0.43
2:S2:433:A:H5''	9:SI:22:HIS:HB3	2.01	0.43
2:S2:628:A:OP2	5:SD:178:ARG:NH1	2.51	0.43
2:S2:1291:A:OP2	2:S2:1302:G:O2'	2.34	0.43
2:S2:1543:U:P	16:ST:62:ARG:HH22	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:SL:59:LYS:HG2	11:SL:134:LEU:HD22	2.00	0.43
23:Sg:193:GLY:HA3	23:Sg:212:LYS:HB3	2.00	0.43
2:S2:563:G:N7	2:S2:586:G:N2	2.66	0.43
2:S2:1845:A:H2'	2:S2:1846:G:C8	2.53	0.43
5:SD:173:ARG:HA	5:SD:173:ARG:HD3	1.86	0.43
7:SF:142:SER:OG	21:Sc:49:PRO:O	2.30	0.43
32:SZ:46:ASN:HB3	32:SZ:80:ARG:HA	2.00	0.43
2:S2:1337:C:H2'	2:S2:1338:G:H8	1.83	0.43
2:S2:1405:A:H2'	2:S2:1406:G:O4'	2.19	0.43
2:S2:1468:C:H2'	2:S2:1469:A:H8	1.83	0.43
2:S2:1865:C:H1'	20:Sa:7:ASN:HD21	1.84	0.43
6:SE:137:PRO:HG2	6:SE:150:PRO:HD2	2.01	0.43
2:S2:795:A:H2'	2:S2:796:G:C8	2.53	0.43
3:SA:128:ARG:NH1	3:SA:151:ASP:OD1	2.52	0.43
6:SE:44:LEU:HD13	6:SE:82:TYR:HB3	2.01	0.43
6:SE:128:LYS:HB2	6:SE:128:LYS:HE3	1.70	0.43
8:SH:15:LYS:HA	8:SH:15:LYS:HD3	1.86	0.43
32:SZ:88:LEU:HD23	32:SZ:109:TYR:CD2	2.54	0.43
11:SL:74:SER:O	11:SL:90:ARG:NH1	2.52	0.43
13:SQ:9:SER:OG	13:SQ:24:HIS:NE2	2.37	0.43
23:Sg:178:ASN:OD1	23:Sg:179:LEU:N	2.52	0.43
23:Sg:245:ARG:HD2	23:Sg:247:TRP:CD2	2.54	0.43
25:SG:5:ILE:HD13	25:SG:111:LEU:HB2	2.01	0.43
2:S2:857:U:H2'	2:S2:858:A:H8	1.84	0.43
2:S2:879:C:N4	2:S2:908:A:N6	2.66	0.43
2:S2:954:U:O2	2:S2:972:A:N7	2.52	0.43
2:S2:1660:C:H4'	2:S2:1663:A:H62	1.83	0.43
7:SF:80:GLY:HA2	7:SF:83:ASN:HB2	2.00	0.43
2:S2:161:U:H5'	31:SY:116:LYS:HD3	2.01	0.43
2:S2:303:C:O2	9:SI:184:ARG:NH1	2.51	0.43
2:S2:1215:C:O2'	2:S2:1645:C:OP2	2.29	0.43
2:S2:1329:U:O2'	2:S2:1332:A:OP2	2.30	0.43
2:S2:1810:U:H2'	2:S2:1811:C:C6	2.54	0.43
12:SP:28:MET:HB3	12:SP:32:GLN:HB2	2.00	0.43
13:SQ:13:PHE:HA	13:SQ:22:VAL:HA	2.01	0.43
2:S2:656:G:H21	2:S2:663:C:H5''	1.83	0.42
2:S2:793:G:H2'	2:S2:794:A:H8	1.84	0.42
2:S2:1106:C:H5''	33:Sb:70:LYS:HE3	2.00	0.42
2:S2:1486:A:H2'	2:S2:1487:A:H8	1.84	0.42
2:S2:1692:U:H2'	2:S2:1693:G:H8	1.83	0.42
23:Sg:4:GLN:O	23:Sg:313:THR:OG1	2.30	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Sg:32:LEU:HD21	23:Sg:92:LEU:HD21	2.02	0.42
23:Sg:129:ILE:HG13	23:Sg:151:VAL:HG11	2.01	0.42
26:SJ:112:THR:HG22	26:SJ:123:ILE:HD11	2.01	0.42
26:SJ:169:ARG:HA	26:SJ:169:ARG:HD2	1.71	0.42
30:SW:25:VAL:HG22	30:SW:63:VAL:HG22	2.01	0.42
33:Sb:49:HIS:O	33:Sb:51:GLN:NE2	2.52	0.42
2:S2:681:U:H4'	19:SX:9:THR:HG22	2.01	0.42
2:S2:1013:U:OP1	2:S2:1129:G:O2'	2.36	0.42
2:S2:1277:C:H2'	2:S2:1278:A:C8	2.54	0.42
2:S2:1601:A:OP2	2:S2:1636:G:N2	2.50	0.42
31:SY:100:LYS:HD2	31:SY:100:LYS:HA	1.84	0.42
35:Sf:118:ARG:HB2	35:Sf:131:PHE:CD2	2.54	0.42
2:S2:906:U:H2'	2:S2:907:G:C8	2.51	0.42
9:SI:162:LEU:HD11	9:SI:191:GLU:HG2	2.01	0.42
13:SQ:93:VAL:HG21	13:SQ:120:LEU:HD21	2.01	0.42
25:SG:32:MET:HE2	25:SG:65:GLN:HB2	2.01	0.42
28:SN:132:LYS:HD3	28:SN:132:LYS:HA	1.88	0.42
30:SW:115:GLU:HA	30:SW:118:ARG:HB2	2.01	0.42
2:S2:795:A:H2'	2:S2:796:G:H8	1.84	0.42
2:S2:819:G:OP1	26:SJ:79:ARG:NH1	2.52	0.42
2:S2:851:C:H5''	2:S2:852:G:H5'	2.00	0.42
2:S2:1172:U:H2'	2:S2:1173:A:H8	1.85	0.42
2:S2:1736:G:H2'	2:S2:1737:G:H8	1.84	0.42
2:S2:1842:C:H2'	2:S2:1843:G:C8	2.54	0.42
4:SB:33:VAL:HG23	4:SB:44:ILE:HB	2.01	0.42
4:SB:107:ARG:NH2	29:SO:133:THR:O	2.52	0.42
15:SS:91:LYS:HE2	15:SS:91:LYS:HB2	1.76	0.42
19:SX:60:LYS:H	19:SX:114:ASP:HB2	1.84	0.42
2:S2:295:C:H2'	2:S2:296:U:C6	2.53	0.42
2:S2:747:U:O4	2:S2:796:G:O6	2.37	0.42
2:S2:1213:C:H2'	2:S2:1214:A:C8	2.54	0.42
2:S2:1630:A:OP1	15:SS:40:TYR:N	2.37	0.42
2:S2:1850:A:H2'	2:S2:1851:A:C8	2.54	0.42
2:S2:984:C:H2'	2:S2:985:G:C8	2.55	0.42
2:S2:1689:C:H2'	2:S2:1690:U:H6	1.84	0.42
17:SU:85:HIS:HB3	17:SU:87:ARG:HH12	1.83	0.42
2:S2:570:C:H4'	31:SY:36:PRO:HB3	2.01	0.42
2:S2:639:C:H2'	2:S2:640:A:H8	1.84	0.42
2:S2:1610:G:HO2'	15:SS:86:ARG:HH21	1.65	0.42
15:SS:86:ARG:HH22	15:SS:110:ASP:CG	2.27	0.42
23:Sg:72:SER:OG	23:Sg:74:ASP:OD1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:SC:94:ILE:HG23	24:SC:98:LEU:HD12	2.02	0.42
2:S2:28:U:H2'	2:S2:29:G:C8	2.54	0.42
2:S2:1093:A:H2'	2:S2:1094:C:C6	2.54	0.42
2:S2:1203:G:H2'	2:S2:1204:A:C8	2.55	0.42
4:SB:42:ARG:NH2	4:SB:232:HIS:O	2.44	0.42
7:SF:165:ASN:OD1	7:SF:166:ILE:N	2.52	0.42
9:SI:67:TRP:NE1	9:SI:191:GLU:OE2	2.53	0.42
9:SI:97:VAL:HG22	9:SI:98:LYS:H	1.85	0.42
10:SK:20:VAL:HG12	10:SK:70:TYR:HA	2.02	0.42
26:SJ:114:VAL:HG21	26:SJ:135:ILE:HG12	2.01	0.42
30:SW:42:MET:HE2	30:SW:50:PHE:HE1	1.85	0.42
33:Sb:11:SER:OG	33:Sb:13:GLU:OE1	2.38	0.42
34:Se:51:LYS:HE2	36:JD:606:LEU:HB3	2.02	0.42
2:S2:555:A:C6	2:S2:557:U:N3	2.88	0.42
2:S2:656:G:H5'	2:S2:662:G:N2	2.35	0.42
2:S2:862:A:C8	30:SW:107:SER:HA	2.55	0.42
21:Sc:5:ARG:O	21:Sc:5:ARG:NH1	2.52	0.42
2:S2:51:U:H2'	2:S2:52:G:C8	2.55	0.42
2:S2:600:G:H2'	2:S2:601:G:C8	2.55	0.42
2:S2:980:A:H2'	2:S2:981:A:C8	2.55	0.42
2:S2:1513:C:OP1	22:Sd:12:ARG:NH1	2.33	0.42
15:SS:113:ARG:O	15:SS:117:ILE:HG12	2.20	0.42
20:Sa:98:PRO:HA	20:Sa:99:PRO:HD3	1.91	0.42
28:SN:47:PRO:HG3	28:SN:75:LEU:HD12	2.01	0.42
2:S2:655:A:H4'	2:S2:656:G:H3'	2.02	0.41
2:S2:693:A:C5	2:S2:739:C:H4'	2.55	0.41
2:S2:1270:G:O2'	2:S2:1301:A:N7	2.49	0.41
2:S2:1808:U:H2'	2:S2:1809:A:C8	2.54	0.41
25:SG:5:ILE:HG22	25:SG:124:LEU:HD21	2.01	0.41
2:S2:375:U:H2'	2:S2:376:A:C8	2.55	0.41
2:S2:1523:C:H2'	2:S2:1524:G:H8	1.84	0.41
6:SE:125:LYS:HE3	6:SE:125:LYS:HB2	1.89	0.41
8:SH:12:ASN:OD1	8:SH:13:GLY:N	2.52	0.41
9:SI:122:GLY:HA2	9:SI:167:GLN:HG2	2.01	0.41
33:Sb:8:LEU:HD12	33:Sb:8:LEU:HA	1.84	0.41
2:S2:374:G:H2'	2:S2:375:U:C6	2.55	0.41
2:S2:1757:G:H8	2:S2:1758:G:H1'	1.85	0.41
4:SB:59:SER:HB2	4:SB:91:VAL:HG21	2.01	0.41
25:SG:2:LYS:HB3	25:SG:15:LEU:HD11	2.02	0.41
26:SJ:92:MET:O	26:SJ:93:LYS:HD2	2.20	0.41
2:S2:1084:A:OP1	2:S2:1858:G:O2'	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S2:1834:A:N6	2:S2:1836:G:H22	2.17	0.41
10:SK:95:ARG:NH2	10:SK:97:SER:O	2.54	0.41
23:Sg:46:THR:OG1	23:Sg:48:ASP:OD1	2.29	0.41
2:S2:639:C:H2'	2:S2:640:A:C8	2.55	0.41
2:S2:1123:C:H4'	4:SB:149:GLN:HG3	2.02	0.41
2:S2:1575:G:H2'	2:S2:1576:G:H8	1.85	0.41
4:SB:98:THR:OG1	4:SB:99:ASN:N	2.52	0.41
4:SB:160:GLN:O	4:SB:164:ILE:HG13	2.20	0.41
5:SD:227:LYS:HD2	5:SD:227:LYS:HA	1.80	0.41
9:SI:113:TYR:HD2	9:SI:121:LEU:HD22	1.85	0.41
35:Sf:139:HIS:N	35:Sf:148:TYR:O	2.53	0.41
2:S2:293:C:O2'	2:S2:294:U:H3'	2.20	0.41
2:S2:389:A:H2'	2:S2:390:C:C6	2.56	0.41
5:SD:23:GLU:HG2	10:SK:64:TRP:HE1	1.86	0.41
9:SI:82:VAL:HG22	9:SI:202:ILE:HD12	2.01	0.41
23:Sg:40:ILE:HB	23:Sg:59:LEU:HB2	2.02	0.41
2:S2:634:A:H2'	2:S2:635:G:H8	1.85	0.41
2:S2:878:G:C6	2:S2:908:A:N1	2.88	0.41
2:S2:1275:G:H22	2:S2:1506:A:P	2.44	0.41
2:S2:1598:G:N7	32:SZ:85:ARG:NH1	2.68	0.41
5:SD:215:ASP:OD1	5:SD:215:ASP:N	2.53	0.41
10:SK:61:GLN:O	10:SK:68:TYR:N	2.51	0.41
13:SQ:26:LYS:HG2	13:SQ:67:ASP:HB2	2.01	0.41
16:ST:52:TRP:HZ3	16:ST:99:VAL:HG21	1.85	0.41
2:S2:1:U:N3	2:S2:3:C:N4	2.69	0.41
2:S2:532:C:C2	2:S2:552:G:C2	3.06	0.41
2:S2:661:U:OP2	19:SX:3:LYS:NZ	2.52	0.41
20:Sa:23:CYS:HB3	20:Sa:28:ARG:H	1.86	0.41
27:SM:55:ASN:OD1	27:SM:82:ASN:N	2.54	0.41
27:SM:60:MET:SD	27:SM:60:MET:N	2.93	0.41
2:S2:12:U:H2'	2:S2:13:C:C6	2.56	0.41
2:S2:51:U:H2'	2:S2:52:G:H8	1.86	0.41
2:S2:158:A:H2'	2:S2:159:A:O4'	2.21	0.41
2:S2:169:U:H5''	25:SG:135:PRO:HA	2.02	0.41
2:S2:562:U:H2'	2:S2:563:G:C8	2.55	0.41
2:S2:696:G:H21	2:S2:737:G:H22	1.67	0.41
2:S2:879:C:N4	2:S2:908:A:H61	2.18	0.41
2:S2:1232:U:H2'	2:S2:1233:G:C8	2.55	0.41
2:S2:1665:G:C5	16:ST:88:MET:HE1	2.55	0.41
3:SA:69:GLU:CD	24:SC:267:GLN:HE21	2.29	0.41
4:SB:147:ASN:OD1	4:SB:148:ASN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:SP:123:TYR:OH	15:SS:124:ARG:NH1	2.50	0.41
13:SQ:42:ILE:HD12	13:SQ:42:ILE:HA	1.95	0.41
13:SQ:134:GLY:HA3	13:SQ:140:ARG:HA	2.02	0.41
18:SV:1:MET:HB3	18:SV:10:ASP:HB2	2.03	0.41
19:SX:48:LYS:HE3	19:SX:48:LYS:HB2	1.90	0.41
20:Sa:33:ASP:N	20:Sa:33:ASP:OD1	2.54	0.41
23:Sg:10:THR:HG22	23:Sg:308:ARG:HG3	2.03	0.41
25:SG:221:LYS:HD2	25:SG:221:LYS:HA	1.95	0.41
29:SO:56:VAL:HG23	29:SO:60:MET:HG3	2.03	0.41
32:SZ:52:LYS:HB2	32:SZ:52:LYS:HE2	1.82	0.41
2:S2:549:C:H2'	2:S2:550:C:C6	2.56	0.41
2:S2:941:C:H2'	2:S2:942:G:C8	2.56	0.41
2:S2:1337:C:H2'	2:S2:1338:G:C8	2.56	0.41
15:SS:60:THR:OG1	15:SS:62:ASP:OD1	2.33	0.41
31:SY:57:VAL:HA	31:SY:73:GLY:HA2	2.02	0.41
2:S2:919:A:H5''	28:SN:16:LEU:HD23	2.01	0.40
2:S2:1468:C:H2'	2:S2:1469:A:C8	2.56	0.40
2:S2:1632:G:OP1	15:SS:34:LYS:NZ	2.53	0.40
4:SB:103:MET:HE1	4:SB:212:VAL:HG13	2.03	0.40
7:SF:110:GLN:HA	7:SF:113:VAL:HG22	2.03	0.40
8:SH:146:VAL:HG12	30:SW:42:MET:HE1	2.03	0.40
12:SP:96:VAL:HG13	12:SP:120:SER:HB2	2.02	0.40
19:SX:124:LYS:HA	19:SX:129:SER:HA	2.03	0.40
23:Sg:183:LYS:O	23:Sg:185:LYS:NZ	2.51	0.40
23:Sg:210:GLY:HA3	23:Sg:236:ILE:HG21	2.04	0.40
25:SG:93:LYS:HB2	25:SG:93:LYS:HE2	1.85	0.40
2:S2:441:C:H2'	2:S2:442:C:C6	2.56	0.40
2:S2:496:C:OP1	6:SE:49:ARG:NH2	2.39	0.40
2:S2:1430:C:H2'	2:S2:1431:G:C8	2.57	0.40
2:S2:1692:U:H2'	2:S2:1693:G:C8	2.56	0.40
2:S2:1777:G:H2'	2:S2:1778:C:C6	2.57	0.40
3:SA:222:VAL:HG23	3:SA:223:THR:HG23	2.02	0.40
8:SH:36:LEU:HD21	8:SH:79:LEU:HD23	2.04	0.40
10:SK:80:ARG:NH1	10:SK:86:PRO:O	2.53	0.40
11:SL:77:VAL:HG12	11:SL:88:ILE:HG22	2.02	0.40
13:SQ:39:LEU:HD11	13:SQ:51:LEU:HG	2.03	0.40
15:SS:86:ARG:NH2	15:SS:110:ASP:OD2	2.47	0.40
23:Sg:49:GLU:C	23:Sg:50:THR:HG1	2.27	0.40
25:SG:5:ILE:HG21	25:SG:45:TRP:HH2	1.87	0.40
2:S2:17:C:H2'	2:S2:18:C:C6	2.56	0.40
2:S2:115:U:H2'	2:S2:116:U:C6	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S2:879:C:H42	2:S2:908:A:N6	2.18	0.40
2:S2:1521:C:OP2	15:SS:124:ARG:NH2	2.44	0.40
2:S2:1546:G:H21	2:S2:1670:C:H1'	1.87	0.40
14:SR:60:ARG:HH21	14:SR:66:VAL:HG21	1.86	0.40
30:SW:84:LYS:HE2	30:SW:84:LYS:HB3	1.87	0.40
2:S2:694:G:H2'	2:S2:695:C:O4'	2.22	0.40
2:S2:1017:U:H5'	28:SN:55:ARG:HD3	2.02	0.40
2:S2:1562:C:H2'	2:S2:1563:G:H8	1.86	0.40
2:S2:1805:G:H2'	2:S2:1806:A:C8	2.56	0.40
5:SD:59:LEU:HA	5:SD:66:ILE:HG23	2.04	0.40
5:SD:213:PRO:HB3	14:SR:20:TYR:HE1	1.87	0.40
9:SI:2:GLY:O	9:SI:24:LYS:NZ	2.54	0.40
9:SI:101:ILE:HD12	9:SI:190:LEU:HD11	2.04	0.40
26:SJ:128:VAL:HG22	26:SJ:132:GLN:HE22	1.86	0.40
28:SN:26:LEU:HD12	28:SN:26:LEU:HA	1.91	0.40
31:SY:7:ILE:HG21	31:SY:43:LYS:HB3	2.03	0.40
36:JD:639:SER:H	36:JD:642:GLN:NE2	2.20	0.40
2:S2:223:C:H2'	2:S2:224:A:C8	2.57	0.40
2:S2:1146:C:O2'	2:S2:1150:A:N1	2.52	0.40
2:S2:1203:G:H2'	2:S2:1204:A:H8	1.86	0.40
2:S2:1217:A:H2'	2:S2:1218:C:C6	2.57	0.40
2:S2:1410:C:H2'	2:S2:1411:G:C8	2.57	0.40
2:S2:1743:G:H21	2:S2:1791:A:N6	2.07	0.40
3:SA:124:VAL:N	3:SA:145:ILE:O	2.50	0.40
6:SE:21:ASP:OD1	6:SE:22:LYS:N	2.54	0.40
8:SH:118:ARG:HA	8:SH:121:THR:HG23	2.02	0.40
9:SI:110:ARG:HG2	9:SI:121:LEU:HD21	2.03	0.40
19:SX:51:VAL:HG12	19:SX:72:VAL:HG12	2.02	0.40
27:SM:35:ILE:HA	27:SM:38:ALA:HB3	2.04	0.40
31:SY:18:LEU:HD23	31:SY:18:LEU:HA	1.89	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	220/295 (75%)	216 (98%)	4 (2%)	0	100	100
4	SB	212/264 (80%)	203 (96%)	9 (4%)	0	100	100
5	SD	225/243 (93%)	221 (98%)	4 (2%)	0	100	100
6	SE	260/263 (99%)	252 (97%)	8 (3%)	0	100	100
7	SF	180/204 (88%)	172 (96%)	7 (4%)	1 (1%)	21	56
8	SH	182/194 (94%)	173 (95%)	9 (5%)	0	100	100
9	SI	204/208 (98%)	193 (95%)	11 (5%)	0	100	100
10	SK	96/165 (58%)	89 (93%)	7 (7%)	0	100	100
11	SL	140/158 (89%)	137 (98%)	3 (2%)	0	100	100
12	SP	125/145 (86%)	123 (98%)	2 (2%)	0	100	100
13	SQ	142/146 (97%)	130 (92%)	12 (8%)	0	100	100
14	SR	133/135 (98%)	127 (96%)	6 (4%)	0	100	100
15	SS	143/152 (94%)	138 (96%)	5 (4%)	0	100	100
16	ST	141/145 (97%)	138 (98%)	3 (2%)	0	100	100
17	SU	102/119 (86%)	94 (92%)	7 (7%)	1 (1%)	12	45
18	SV	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
19	SX	139/143 (97%)	133 (96%)	6 (4%)	0	100	100
20	Sa	100/115 (87%)	99 (99%)	1 (1%)	0	100	100
21	Sc	62/69 (90%)	61 (98%)	1 (2%)	0	100	100
22	Sd	53/56 (95%)	49 (92%)	4 (8%)	0	100	100
23	Sg	311/317 (98%)	294 (94%)	15 (5%)	2 (1%)	21	56
24	SC	220/293 (75%)	214 (97%)	6 (3%)	0	100	100
25	SG	235/249 (94%)	224 (95%)	11 (5%)	0	100	100
26	SJ	183/194 (94%)	176 (96%)	7 (4%)	0	100	100
27	SM	120/132 (91%)	111 (92%)	9 (8%)	0	100	100
28	SN	148/151 (98%)	139 (94%)	8 (5%)	1 (1%)	18	52
29	SO	133/151 (88%)	124 (93%)	9 (7%)	0	100	100
30	SW	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
31	SY	123/133 (92%)	119 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	SZ	73/125 (58%)	67 (92%)	6 (8%)	0	100	100
33	Sb	81/84 (96%)	77 (95%)	4 (5%)	0	100	100
34	Se	56/59 (95%)	49 (88%)	7 (12%)	0	100	100
35	Sf	59/156 (38%)	55 (93%)	4 (7%)	0	100	100
36	JD	48/1096 (4%)	47 (98%)	1 (2%)	0	100	100
All	All	4879/6597 (74%)	4665 (96%)	209 (4%)	5 (0%)	49	79

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	SF	80	GLY
23	Sg	50	THR
23	Sg	130	LYS
17	SU	94	PRO
28	SN	68	GLY

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	184/243 (76%)	184 (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	156/170 (92%)	156 (100%)	0	100	100
8	SH	166/174 (95%)	166 (100%)	0	100	100
9	SI	178/180 (99%)	178 (100%)	0	100	100
10	SK	89/136 (65%)	89 (100%)	0	100	100
11	SL	130/142 (92%)	130 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	SP	113/130 (87%)	113 (100%)	0	100	100
13	SQ	119/121 (98%)	119 (100%)	0	100	100
14	SR	122/122 (100%)	121 (99%)	1 (1%)	73	82
15	SS	126/132 (96%)	126 (100%)	0	100	100
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%)	113 (100%)	0	100	100
20	Sa	89/98 (91%)	89 (100%)	0	100	100
21	Sc	57/62 (92%)	56 (98%)	1 (2%)	51	74
22	Sd	48/49 (98%)	48 (100%)	0	100	100
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	105/119 (88%)	105 (100%)	0	100	100
30	SW	112/113 (99%)	112 (100%)	0	100	100
31	SY	109/115 (95%)	109 (100%)	0	100	100
32	SZ	66/103 (64%)	66 (100%)	0	100	100
33	Sb	75/76 (99%)	75 (100%)	0	100	100
34	Se	47/48 (98%)	47 (100%)	0	100	100
35	Sf	54/140 (39%)	54 (100%)	0	100	100
36	JD	46/948 (5%)	46 (100%)	0	100	100
All	All	4270/5632 (76%)	4268 (100%)	2 (0%)	100	100

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

Mol	Chain	Res	Type
14	SR	50	ILE
21	Sc	29	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
3	SA	50	ASN
4	SB	92	GLN
4	SB	95	ASN
4	SB	124	HIS
4	SB	158	HIS
5	SD	4	GLN
7	SF	29	GLN
7	SF	114	ASN
8	SH	68	GLN
8	SH	165	ASN
9	SI	84	ASN
9	SI	116	HIS
9	SI	138	ASN
9	SI	146	GLN
11	SL	39	ASN
13	SQ	11	GLN
13	SQ	48	GLN
13	SQ	77	HIS
13	SQ	86	GLN
14	SR	93	GLN
15	SS	85	ASN
15	SS	134	GLN
16	ST	128	GLN
17	SU	81	GLN
18	SV	2	GLN
19	SX	31	HIS
19	SX	61	GLN
19	SX	97	ASN
23	Sg	20	GLN
23	Sg	76	GLN
23	Sg	119	GLN
23	Sg	296	GLN
27	SM	19	GLN
27	SM	82	ASN
28	SN	62	GLN
29	SO	113	GLN
30	SW	70	ASN
32	SZ	46	ASN
34	Se	39	ASN
36	JD	588	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	S2	1715/1869 (91%)	402 (23%)	6 (0%)

All (402) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	S2	2	A
2	S2	4	C
2	S2	13	C
2	S2	14	C
2	S2	25	A
2	S2	26	U
2	S2	33	G
2	S2	41	G
2	S2	42	A
2	S2	44	U
2	S2	46	A
2	S2	49	C
2	S2	56	G
2	S2	58	C
2	S2	64	A
2	S2	66	G
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	103	A
2	S2	113	G
2	S2	114	G
2	S2	115	U
2	S2	116	U
2	S2	118	C
2	S2	121	U
2	S2	126	G
2	S2	130	G
2	S2	143	U
2	S2	147	A
2	S2	149	A
2	S2	151	C
2	S2	154	U

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Mol	Chain	Res	Type
2	S2	158	A
2	S2	159	A
2	S2	160	U
2	S2	161	U
2	S2	162	C
2	S2	170	A
2	S2	173	A
2	S2	175	A
2	S2	179	C
2	S2	190	G
2	S2	196	C
2	S2	197	U
2	S2	198	U
2	S2	199	C
2	S2	200	G
2	S2	203	G
2	S2	204	G
2	S2	206	G
2	S2	208	G
2	S2	214	U
2	S2	291	G
2	S2	292	A
2	S2	293	C
2	S2	294	U
2	S2	295	C
2	S2	306	C
2	S2	307	G
2	S2	308	G
2	S2	309	G
2	S2	311	C
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	329	G
2	S2	332	G
2	S2	335	G
2	S2	339	A
2	S2	347	G
2	S2	357	C

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Mol	Chain	Res	Type
2	S2	360	A
2	S2	361	U
2	S2	362	C
2	S2	363	A
2	S2	364	A
2	S2	367	U
2	S2	368	U
2	S2	369	C
2	S2	381	C
2	S2	385	G
2	S2	386	C
2	S2	408	A
2	S2	409	C
2	S2	438	G
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	466	G
2	S2	467	G
2	S2	471	G
2	S2	472	C
2	S2	474	G
2	S2	482	G
2	S2	487	U
2	S2	488	U
2	S2	492	C
2	S2	493	A
2	S2	516	A
2	S2	525	A
2	S2	529	A
2	S2	531	A
2	S2	532	C
2	S2	533	A
2	S2	536	A
2	S2	537	C
2	S2	540	U
2	S2	542	U
2	S2	546	G
2	S2	547	G

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Mol	Chain	Res	Type
2	S2	556	U
2	S2	557	U
2	S2	558	G
2	S2	559	G
2	S2	563	G
2	S2	564	A
2	S2	583	C
2	S2	589	G
2	S2	590	A
2	S2	591	U
2	S2	597	G
2	S2	604	A
2	S2	607	U
2	S2	608	C
2	S2	614	C
2	S2	617	G
2	S2	626	G
2	S2	627	U
2	S2	628	A
2	S2	629	A
2	S2	631	U
2	S2	643	A
2	S2	644	G
2	S2	655	A
2	S2	660	C
2	S2	664	A
2	S2	668	A
2	S2	669	A
2	S2	670	A
2	S2	671	A
2	S2	672	A
2	S2	673	G
2	S2	687	C
2	S2	688	U
2	S2	689	U
2	S2	690	G
2	S2	692	G
2	S2	693	A
2	S2	694	G
2	S2	695	C
2	S2	696	G
2	S2	697	G

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Mol	Chain	Res	Type
2	S2	698	G
2	S2	732	U
2	S2	734	C
2	S2	736	C
2	S2	737	G
2	S2	738	C
2	S2	749	U
2	S2	751	G
2	S2	752	G
2	S2	753	C
2	S2	788	G
2	S2	791	C
2	S2	792	C
2	S2	798	A
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	834	C
2	S2	835	C
2	S2	836	G
2	S2	837	A
2	S2	838	G
2	S2	839	C
2	S2	840	C
2	S2	842	C
2	S2	847	A
2	S2	870	A
2	S2	873	G
2	S2	874	G
2	S2	878	G
2	S2	879	C
2	S2	880	G
2	S2	882	U
2	S2	883	U
2	S2	887	U
2	S2	888	U
2	S2	889	U
2	S2	891	G
2	S2	893	U

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Mol	Chain	Res	Type
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	905	C
2	S2	913	A
2	S2	914	U
2	S2	920	A
2	S2	930	C
2	S2	933	G
2	S2	938	A
2	S2	954	U
2	S2	955	A
2	S2	956	G
2	S2	957	A
2	S2	963	A
2	S2	969	U
2	S2	970	G
2	S2	971	G
2	S2	972	A
2	S2	978	G
2	S2	990	A
2	S2	992	A
2	S2	997	A
2	S2	999	G
2	S2	1017	U
2	S2	1023	A
2	S2	1030	A
2	S2	1045	U
2	S2	1061	U
2	S2	1062	A
2	S2	1078	C
2	S2	1083	A
2	S2	1085	C
2	S2	1087	A
2	S2	1089	G
2	S2	1109	C
2	S2	1114	U

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Mol	Chain	Res	Type
2	S2	1115	U
2	S2	1116	C
2	S2	1118	C
2	S2	1133	A
2	S2	1135	C
2	S2	1138	C
2	S2	1153	C
2	S2	1154	U
2	S2	1170	A
2	S2	1182	A
2	S2	1183	A
2	S2	1195	A
2	S2	1208	A
2	S2	1215	C
2	S2	1216	C
2	S2	1217	A
2	S2	1224	G
2	S2	1227	G
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	1263	U
2	S2	1264	C
2	S2	1265	A
2	S2	1271	C
2	S2	1274	G
2	S2	1275	G
2	S2	1283	C
2	S2	1284	A
2	S2	1285	G
2	S2	1286	G
2	S2	1294	G
2	S2	1295	A
2	S2	1301	A
2	S2	1302	G
2	S2	1303	C
2	S2	1304	U
2	S2	1306	U

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Mol	Chain	Res	Type
2	S2	1308	U
2	S2	1312	G
2	S2	1315	U
2	S2	1333	U
2	S2	1348	G
2	S2	1363	C
2	S2	1371	U
2	S2	1372	U
2	S2	1373	C
2	S2	1378	A
2	S2	1397	U
2	S2	1419	C
2	S2	1420	G
2	S2	1421	A
2	S2	1422	G
2	S2	1423	C
2	S2	1424	G
2	S2	1433	C
2	S2	1435	C
2	S2	1436	C
2	S2	1438	A
2	S2	1452	A
2	S2	1454	A
2	S2	1462	U
2	S2	1463	U
2	S2	1464	C
2	S2	1480	A
2	S2	1489	A
2	S2	1490	G
2	S2	1497	G
2	S2	1498	A
2	S2	1505	U
2	S2	1507	G
2	S2	1508	A
2	S2	1509	U
2	S2	1520	G
2	S2	1521	C
2	S2	1522	A
2	S2	1523	C
2	S2	1533	A
2	S2	1534	C
2	S2	1537	A

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Mol	Chain	Res	Type
2	S2	1544	C
2	S2	1552	G
2	S2	1553	C
2	S2	1556	A
2	S2	1570	G
2	S2	1574	C
2	S2	1578	U
2	S2	1580	A
2	S2	1587	G
2	S2	1588	A
2	S2	1594	A
2	S2	1601	A
2	S2	1606	G
2	S2	1621	U
2	S2	1623	A
2	S2	1630	A
2	S2	1634	A
2	S2	1637	A
2	S2	1638	G
2	S2	1639	G
2	S2	1640	A
2	S2	1648	G
2	S2	1654	G
2	S2	1663	A
2	S2	1665	G
2	S2	1671	G
2	S2	1683	C
2	S2	1684	C
2	S2	1695	A
2	S2	1715	A
2	S2	1716	C
2	S2	1719	A
2	S2	1721	U
2	S2	1722	G
2	S2	1742	C
2	S2	1743	G
2	S2	1744	G
2	S2	1745	A
2	S2	1752	C
2	S2	1753	C
2	S2	1754	G
2	S2	1757	G

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Mol	Chain	Res	Type
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	1776	G
2	S2	1777	G
2	S2	1781	A
2	S2	1782	G
2	S2	1783	C
2	S2	1784	G
2	S2	1786	U
2	S2	1798	C
2	S2	1819	A
2	S2	1822	A
2	S2	1823	A
2	S2	1824	A
2	S2	1826	G
2	S2	1829	G
2	S2	1831	A
2	S2	1835	A
2	S2	1838	U
2	S2	1849	G
2	S2	1852	C
2	S2	1861	G
2	S2	1862	G
2	S2	1863	A
2	S2	1864	U
2	S2	1865	C

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	S2	113	G
2	S2	291	G
2	S2	293	C
2	S2	688	U
2	S2	954	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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

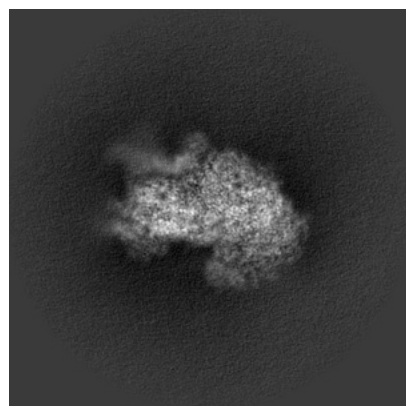
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38548. These allow visual inspection of the internal detail of the map and identification of artifacts.

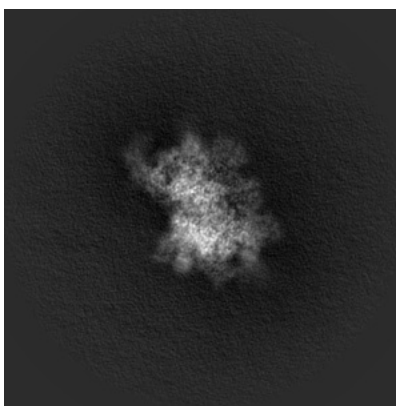
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

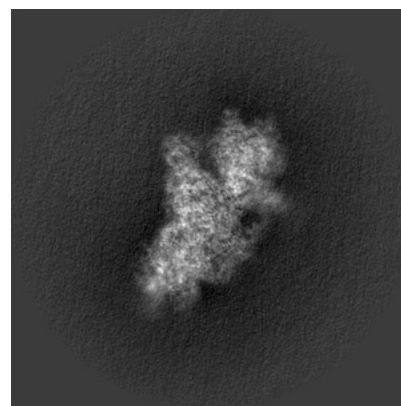
6.1.1 Primary map



X

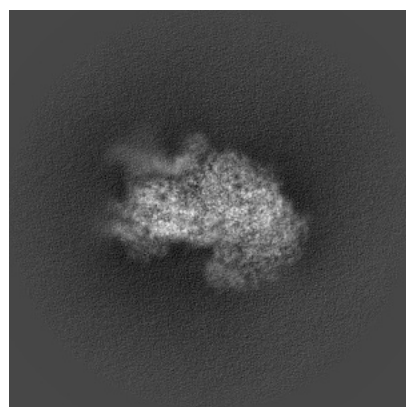


Y

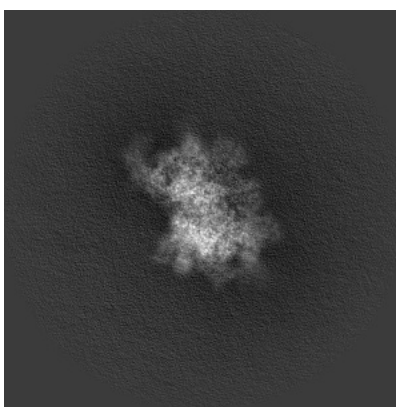


Z

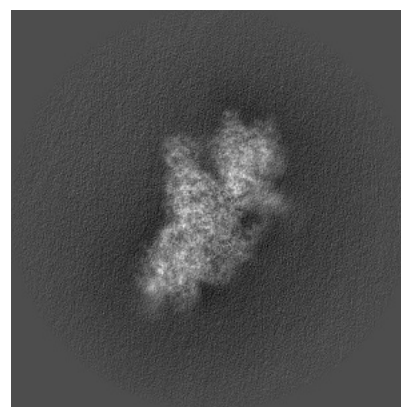
6.1.2 Raw map



X



Y

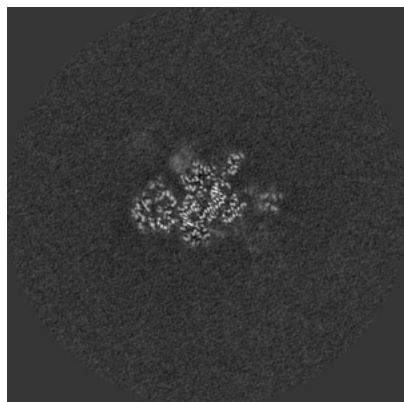


Z

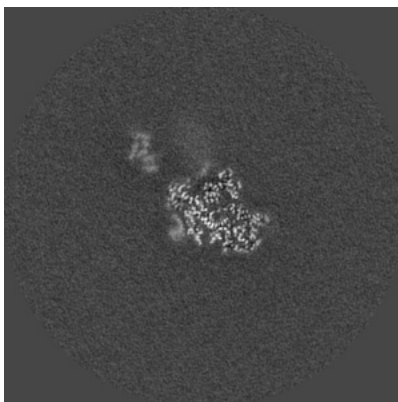
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

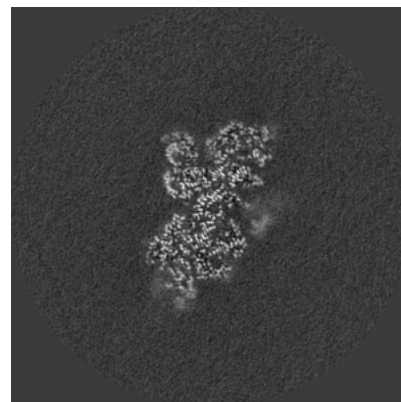
6.2.1 Primary map



X Index: 210

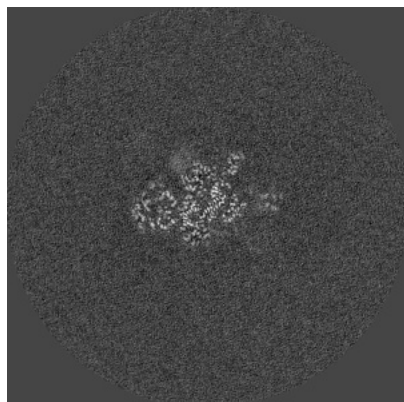


Y Index: 210

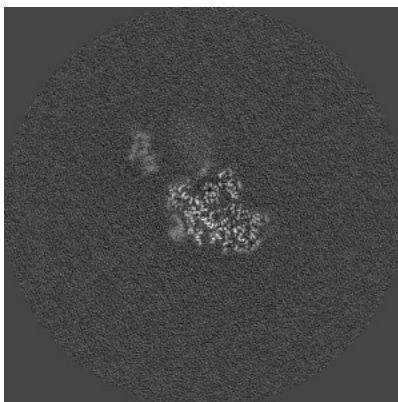


Z Index: 210

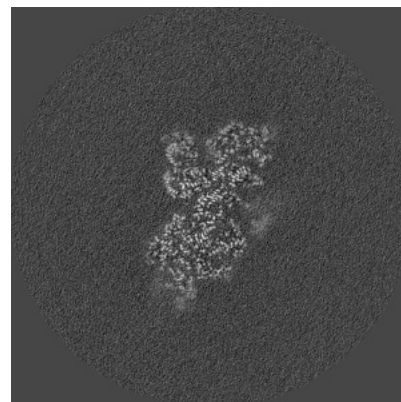
6.2.2 Raw map



X Index: 210



Y Index: 210

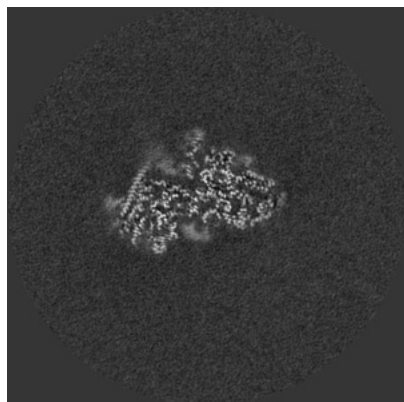


Z Index: 210

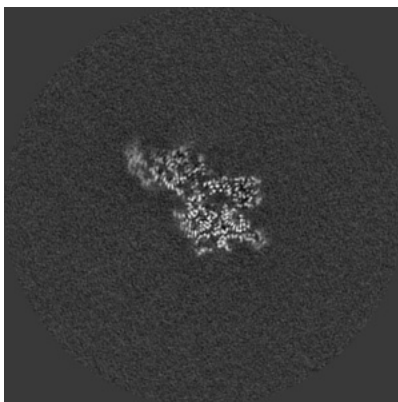
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

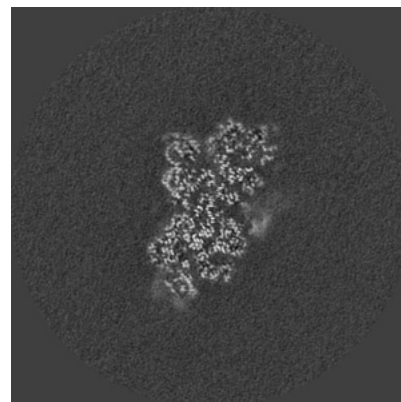
6.3.1 Primary map



X Index: 179

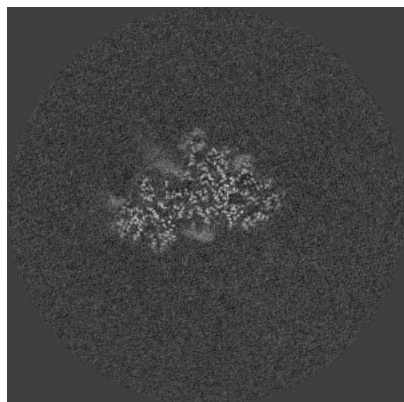


Y Index: 232

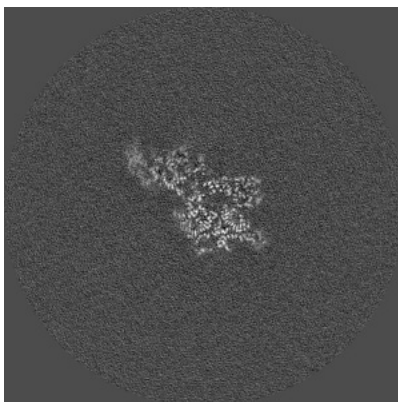


Z Index: 208

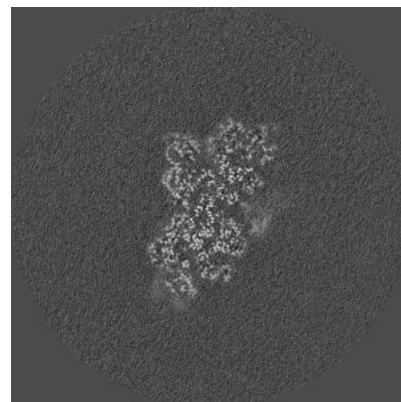
6.3.2 Raw map



X Index: 182



Y Index: 232

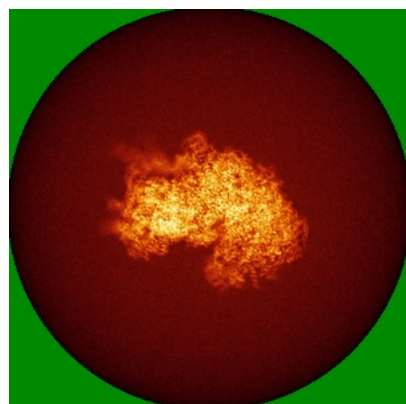


Z Index: 208

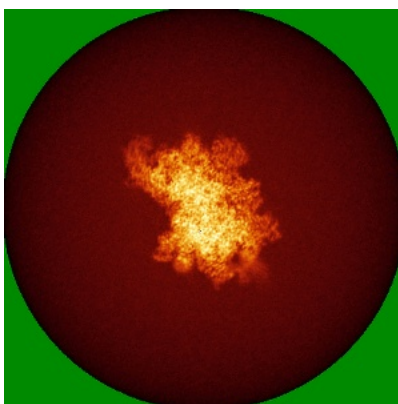
The images above show the largest variance slices of the map in three orthogonal directions.

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

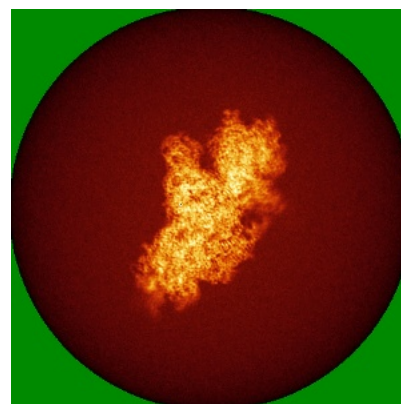
6.4.1 Primary map



X

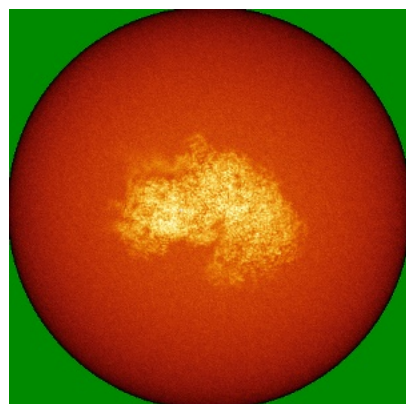


Y

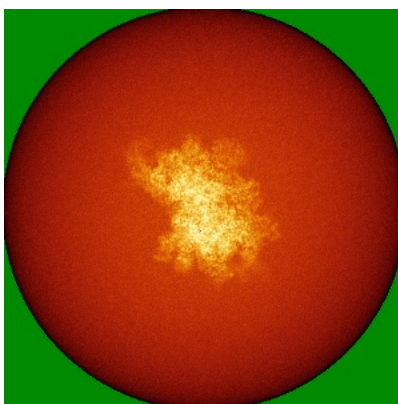


Z

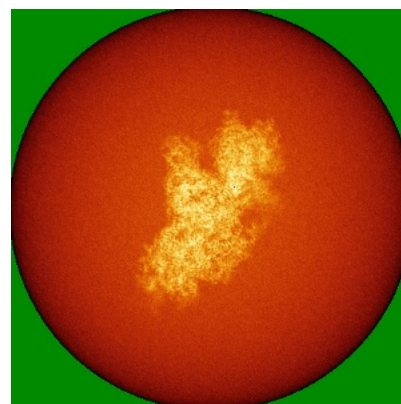
6.4.2 Raw map



X



Y

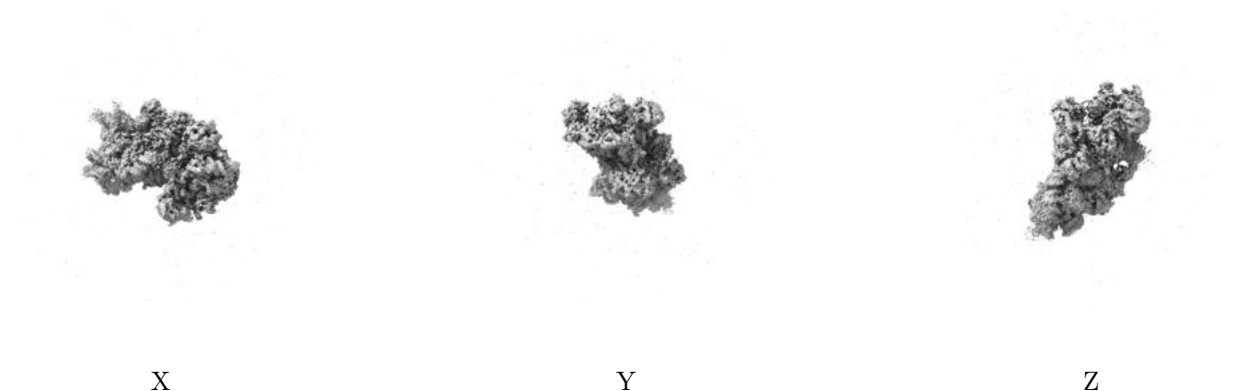


Z

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.

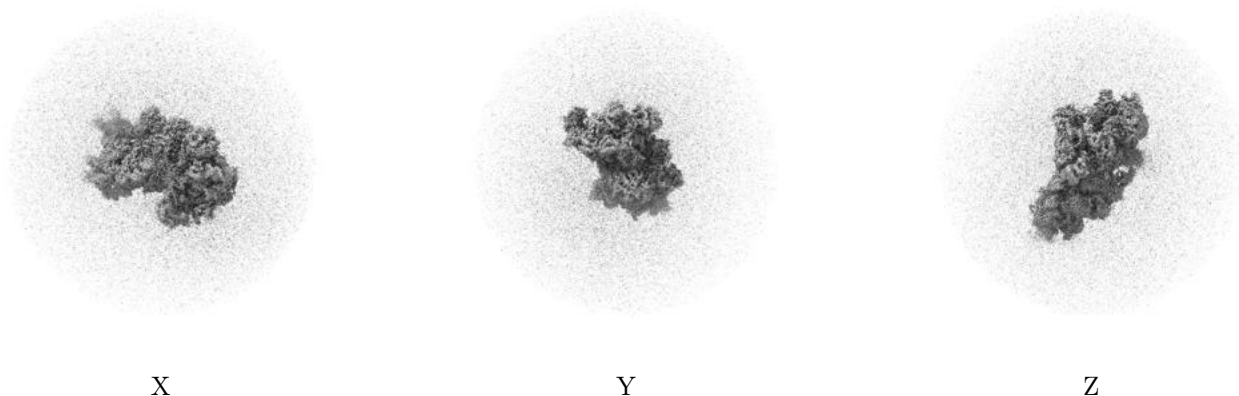
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. 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.

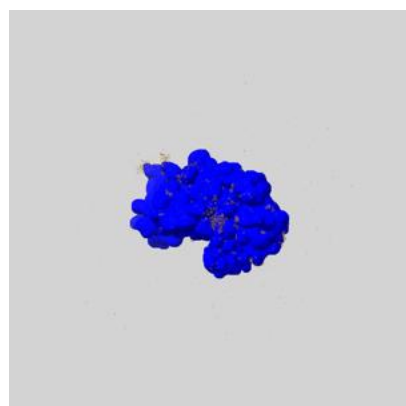
6.6 Mask visualisation [i](#)

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

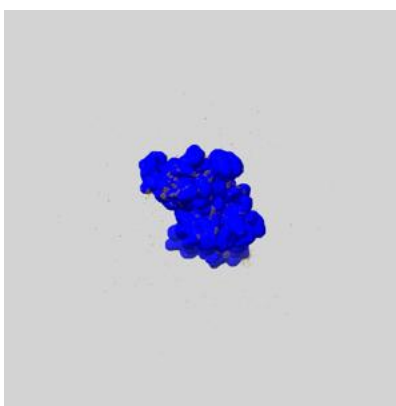
A mask typically either:

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

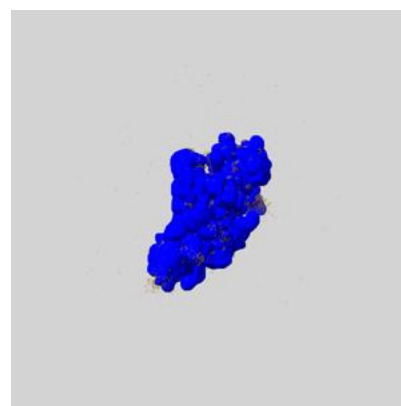
6.6.1 emd_38548_msk_1.map [i](#)



X



Y

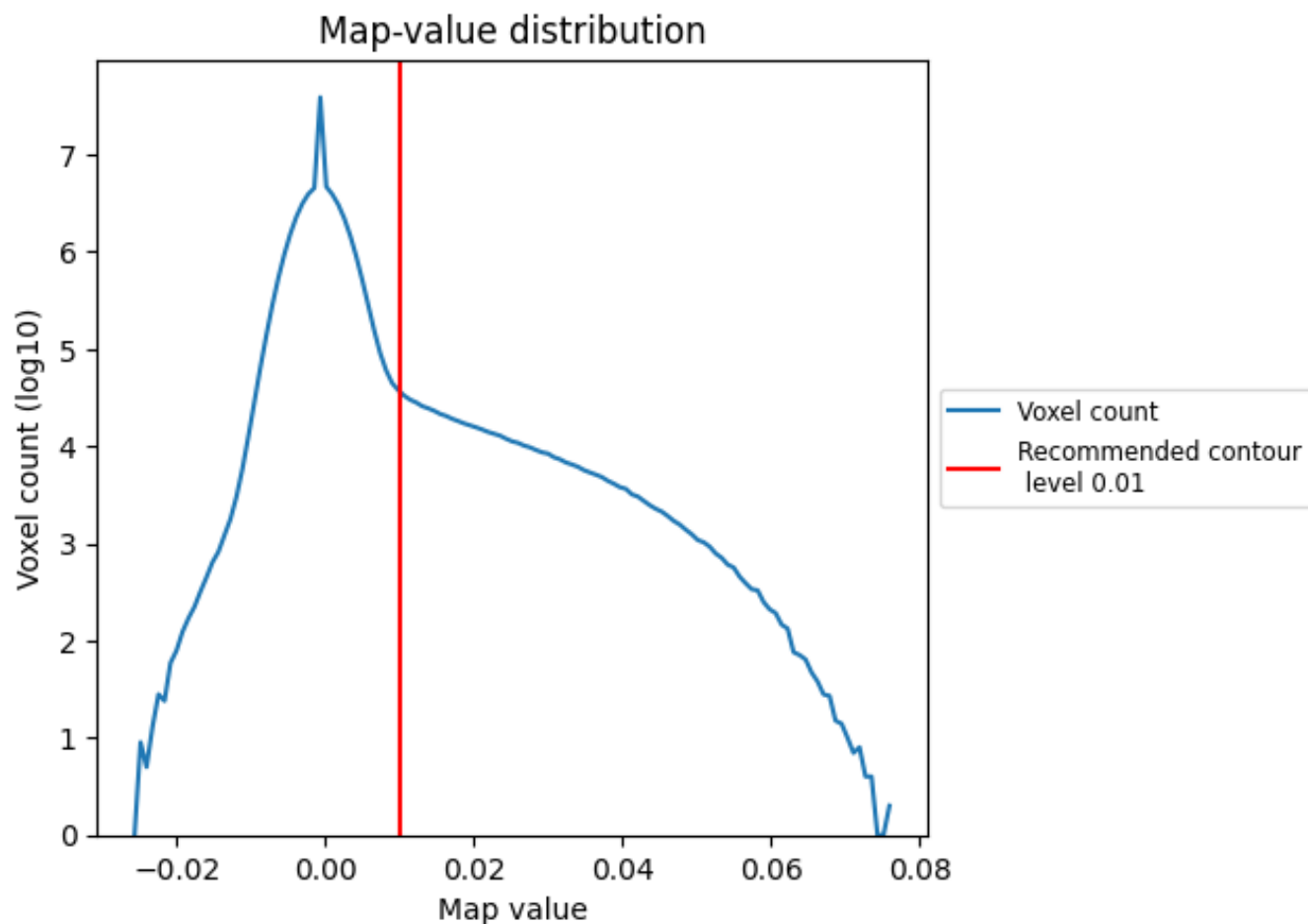


Z

7 Map analysis [i](#)

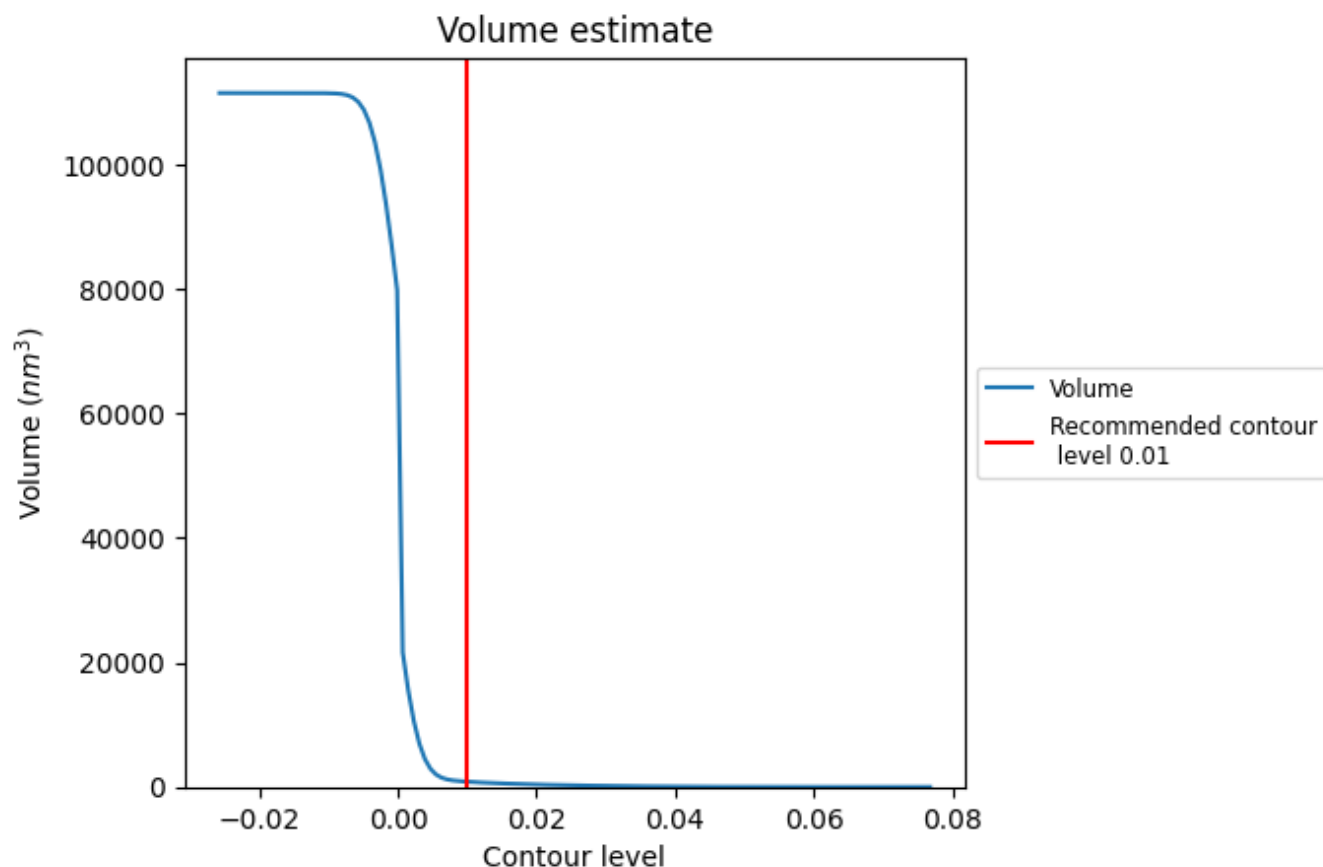
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

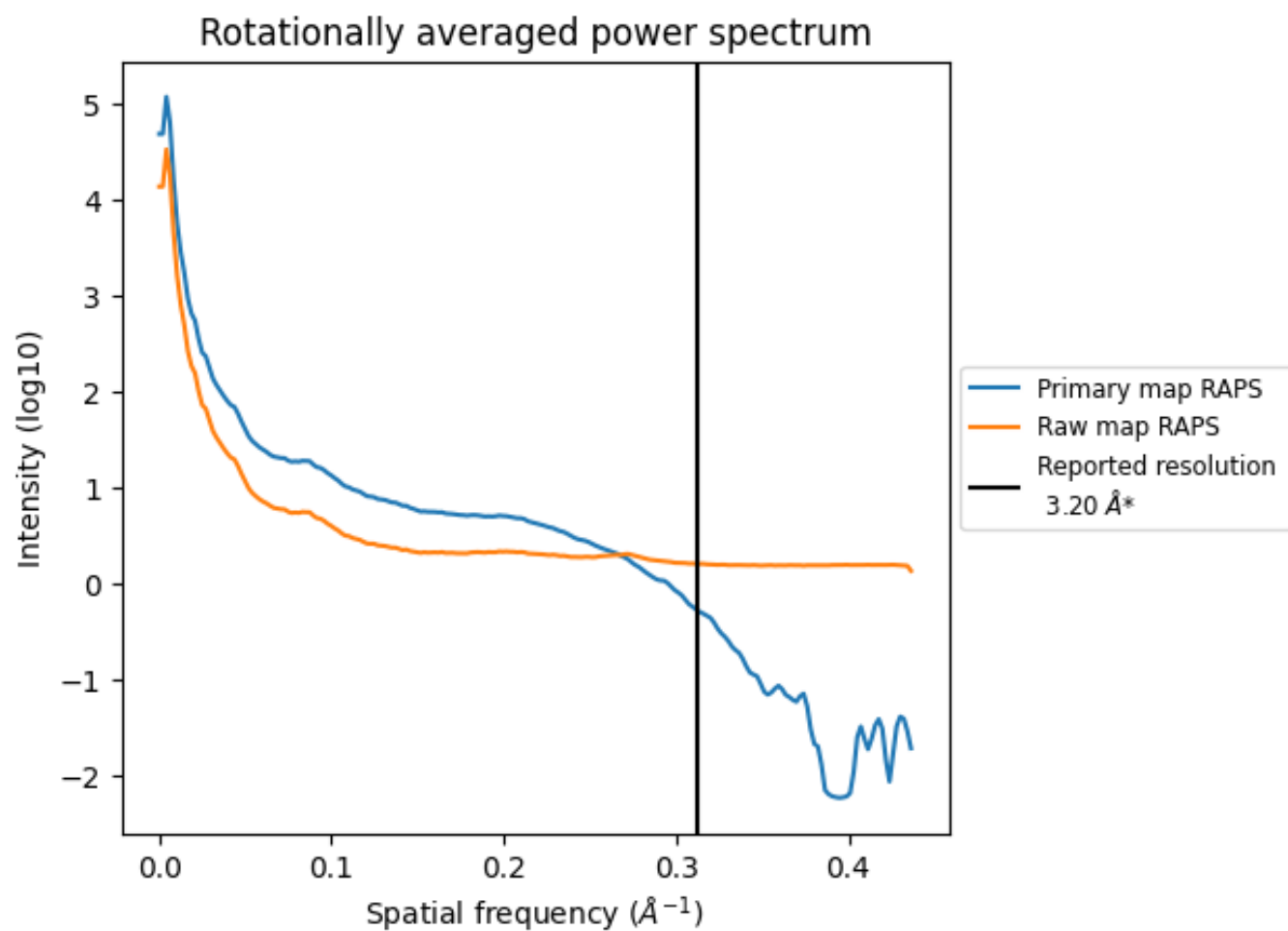
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 843 nm^3 ; this corresponds to an approximate mass of 761 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 ⓘ

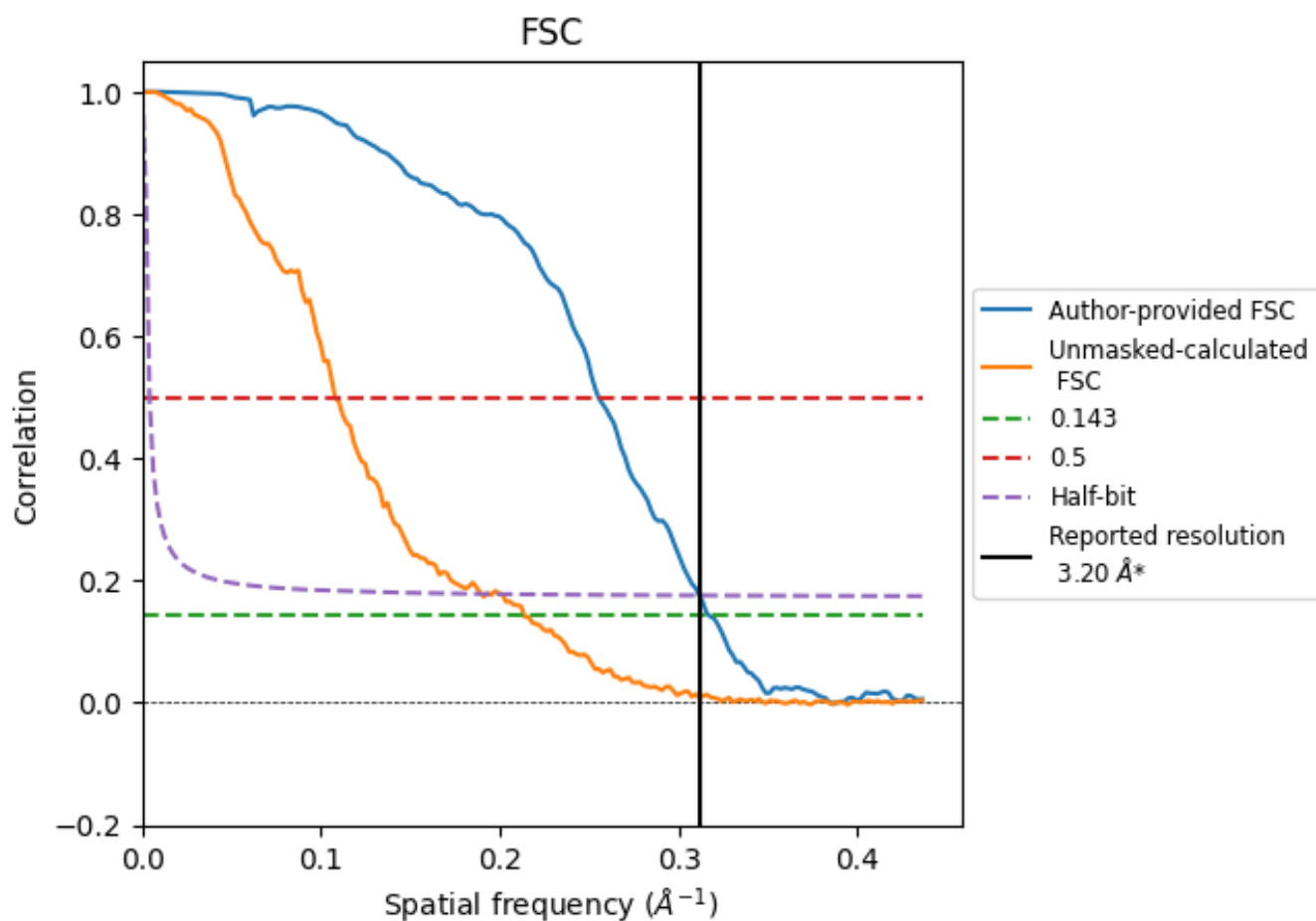


*Reported resolution corresponds to spatial frequency of 0.312 $\text{\AA}^{-1}$

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 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

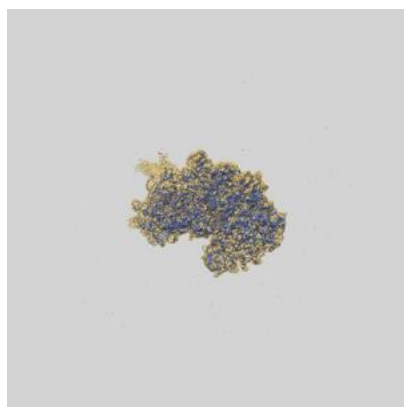
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.15	3.92	3.21
Unmasked-calculated*	4.68	9.27	5.27

*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 4.68 differs from the reported value 3.2 by more than 10 %

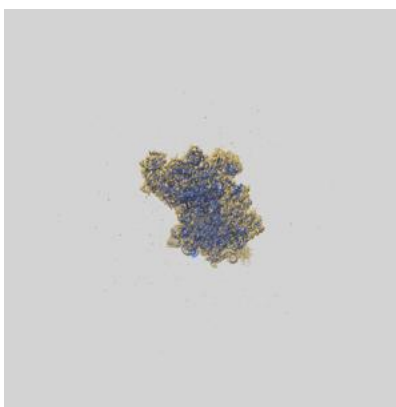
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38548 and PDB model 8XP2. Per-residue inclusion information can be found in section [3](#) on page [11](#).

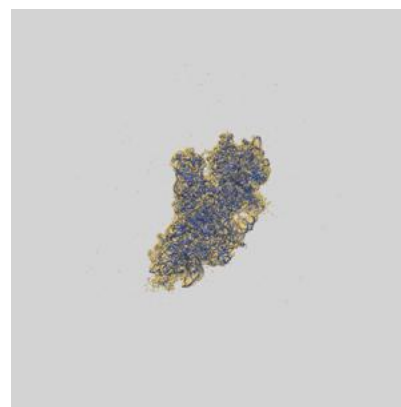
9.1 Map-model overlay [i](#)



X



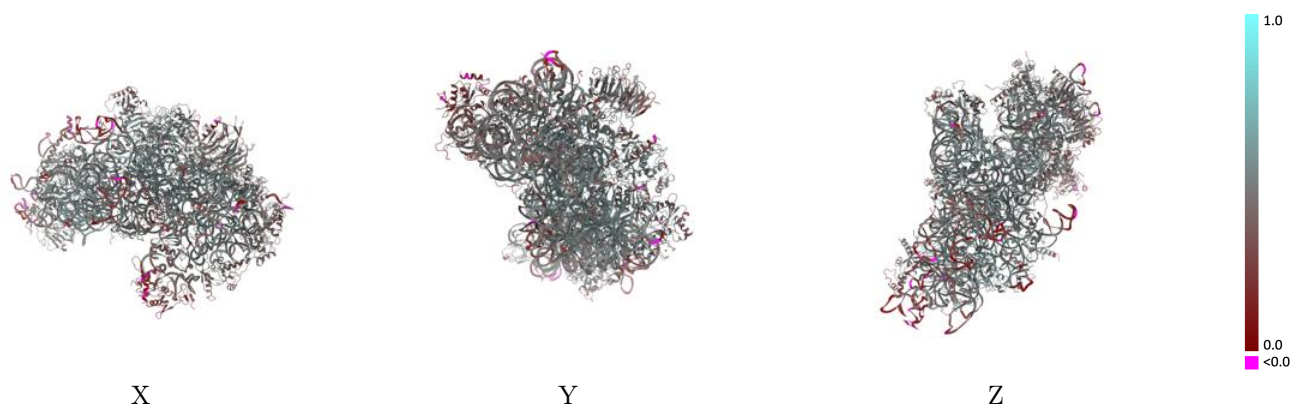
Y



Z

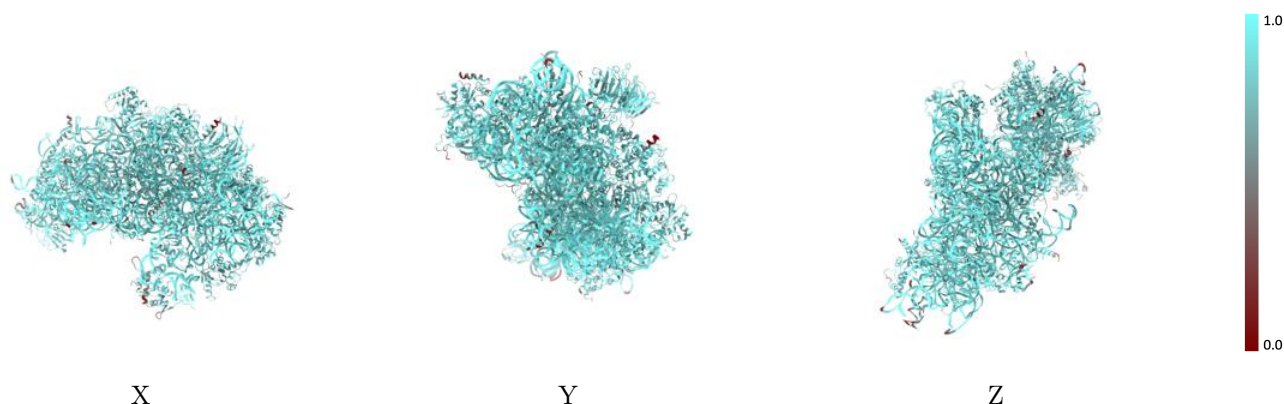
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



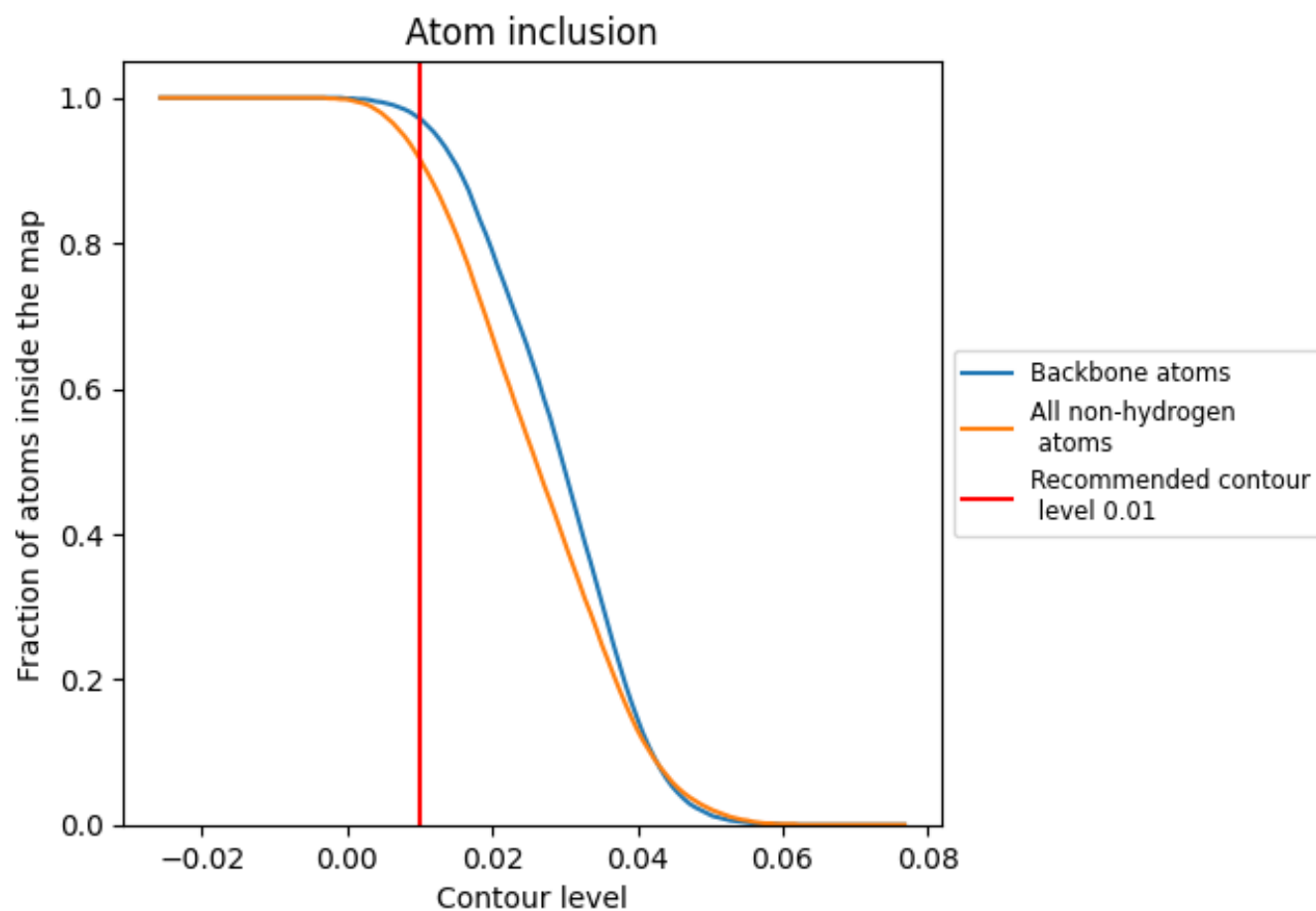
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 92% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9160	 0.4620
JD	 0.6590	 0.3490
Ln	 0.3440	 0.3270
S2	 0.9670	 0.4670
SA	 0.8800	 0.4920
SB	 0.8990	 0.4800
SC	 0.8940	 0.5090
SD	 0.8450	 0.4470
SE	 0.9130	 0.5160
SF	 0.8770	 0.4650
SG	 0.8790	 0.4280
SH	 0.8630	 0.4290
SI	 0.8890	 0.4580
SJ	 0.9040	 0.5000
SK	 0.8440	 0.4000
SL	 0.9170	 0.5080
SM	 0.6950	 0.2440
SN	 0.8940	 0.4810
SO	 0.8840	 0.4800
SP	 0.8060	 0.4170
SQ	 0.8640	 0.4780
SR	 0.8630	 0.4670
SS	 0.8090	 0.4190
ST	 0.8750	 0.4510
SU	 0.8210	 0.4310
SV	 0.9260	 0.5070
SW	 0.9250	 0.5260
SX	 0.9230	 0.5140
SY	 0.9150	 0.4840
SZ	 0.7860	 0.4020
Sa	 0.8860	 0.5070
Sb	 0.8860	 0.4750
Sc	 0.8310	 0.4340
Sd	 0.8890	 0.4880
Se	 0.8110	 0.4260



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Chain	Atom inclusion	Q-score
Sf	 0.7930	 0.2880
Sg	 0.8730	 0.4250