



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:33 PM UTC

PDB ID : 8XXN / pdb_00008xxn
EMDB ID : EMD-38754
Title : Cryo-EM structure of the human 43S ribosome with PDCD4
Authors : Ye, X.; Huang, Z.; Li, Y.; Wang, M.; Cheng, J.
Deposited on : 2024-01-18
Resolution : 3.60 Å(reported)
Based on initial model : 7A09

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

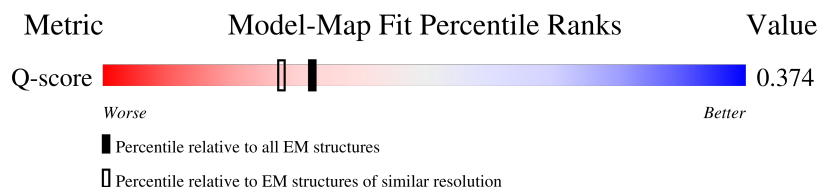
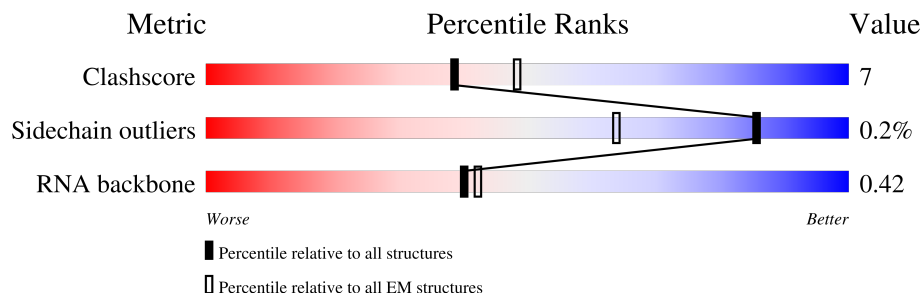
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	
4	SB	264	

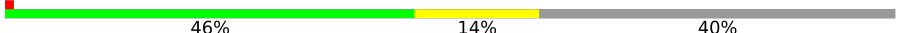
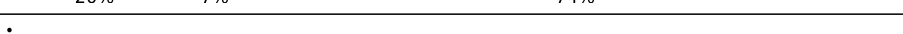
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Mol	Chain	Length	Quality of chain
5	SD	243	
6	SE	263	
7	SF	204	
8	SH	194	
9	SI	208	
10	SK	165	
11	SL	158	
12	SP	145	
13	SQ	146	
14	SR	135	
15	SS	152	
16	ST	145	
17	SU	119	
18	SV	83	
19	SX	143	
20	Sa	115	
21	Sc	69	
22	Sd	56	
23	Sg	317	
24	SC	293	
25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

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Mol	Chain	Length	Quality of chain
30	SW	130	
31	SY	133	
32	SZ	125	
33	Sb	84	
34	Se	59	
35	Sf	156	
36	C1	113	
37	4A	406	
38	CD	469	
39	3A	1382	
40	3B	814	
41	3C	913	
42	3E	445	
43	3F	357	
44	3G	320	
45	3H	352	
46	3I	325	
47	3K	218	
48	3L	564	
49	3M	374	
50	3N	548	

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 114565 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
			36535	16298	6533	11982	1722		

- 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	103	Total	C	N	O	S	0	0
			817	511	155	147	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 Eukaryotic translation initiation factor 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	C1	90	Total	C	N	O	0	0
			443	262	90	91		

- Molecule 37 is a protein called Eukaryotic initiation factor 4A-I.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	4A	342	Total	C	N	O	0	0
			1691	1007	342	342		

- Molecule 38 is a protein called Programmed cell death protein 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	CD	347	Total	C	N	O	0	0
			1841	1100	368	373		

- Molecule 39 is a protein called Eukaryotic translation initiation factor 3 subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	3A	692	Total	C	N	O	S	0	0
			5379	3374	980	1003	22		

- Molecule 40 is a protein called Eukaryotic translation initiation factor 3 subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	3B	536	Total	C	N	O	S	0	0
			2966	1801	580	580	5		

- Molecule 41 is a protein called Eukaryotic translation initiation factor 3 subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	3C	625	Total	C	N	O	S	0	0
			5070	3204	898	933	35		

- Molecule 42 is a protein called Eukaryotic translation initiation factor 3 subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	3E	416	Total	C	N	O	S	0	0
			3437	2202	585	630	20		

- Molecule 43 is a protein called Eukaryotic translation initiation factor 3 subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	3F	269	Total	C	N	O	S	0	0
			2090	1317	356	405	12		

- Molecule 44 is a protein called Eukaryotic translation initiation factor 3 subunit G.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	3G	84	Total	C	N	O		0	0
			667	418	120	129			

- Molecule 45 is a protein called Eukaryotic translation initiation factor 3 subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	3H	295	Total	C	N	O	S	0	0
			2413	1532	417	449	15		

- Molecule 46 is a protein called Eukaryotic translation initiation factor 3 subunit I.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	3I	305	Total	C	N	O		0	0
			1497	887	305	305			

- Molecule 47 is a protein called Eukaryotic translation initiation factor 3 subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	3K	217	Total	C	N	O	S	0	0
			1750	1116	288	334	12		

- Molecule 48 is a protein called Eukaryotic translation initiation factor 3 subunit L.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	3L	372	Total	C	N	O	S	0	0
			3111	2011	520	563	17		

- Molecule 49 is a protein called Eukaryotic translation initiation factor 3 subunit M.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	3M	338	Total	C	N	O	S	0	0
			2705	1727	457	504	17		

- Molecule 50 is a protein called Eukaryotic translation initiation factor 3 subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	3N	447	Total	C	N	O	S	0	0
			3617	2279	625	691	22		

- Molecule 51 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
51	S2	22	Total	Mg	0
			22	22	
51	SG	1	Total	Mg	0
			1	1	

- Molecule 52 is ZINC ION (CCD ID: ZN) (formula: Zn).

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



SER VAL PRO PRO ILE GLN GLN PHE PRO THR GLU ASP TRP SER GLN PRO GLY THR ASP TRP SER

• Molecule 4: 40S ribosomal protein S3a

Chain SB:  67% 14% 19%

MET ALA VAL GLY LYS ASN PHE ARG LEU THR LYS ASP TRP SER GLN PRO GLY THR ASP TRP SER
 R151 K152 Y155 R162 E175 P190 D191 S192 I193 E198 V210 K214 K222 F223 E224 K227 H232 G233 E234 GLY SER SER GLY LYS ALA THR GLY ASP THR R82 K83 F84 C96 L97 R107 Q118 T119 H124 L137 T143 K144 K145 I150
 R151 K152 Y155 R162 E175 P190 D191 S192 I193 E198 V210 K214 K222 F223 E224 K227 H232 G233 E234 GLY SER SER GLY LYS ALA THR GLY ASP THR R82 K83 F84 C96 L97 R107 Q118 T119 H124 L137 T143 K144 K145 I150

• Molecule 5: 40S ribosomal protein S3

Chain SD:  78% 15% 7%

H1 G36 T42 R45 T48 L59 R67 T70 R76 S83 L86 Y87 R94 G95 Q101 R106 C119 V122 A131 K132 V136 V137 K151 M157 T170 R173 L177 R178 Q179 V186 K187 I188 M189 L190 P191 T195
 G196 K197 V211 E212 P213 K214 D215 K226 K227 GLY GLY LYS PRO GLU PRO PRO PRO MET PRO GLN PRO VAL PRO THR ALA

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

Chain SE:  84% 15%

MET A2 R11 P15 M19 T24 A28 R39 I45 R51 M66 K71 R76 T77 T78 D79 I80 M87 D88 V89 I92 D93 K94 T105 R108 H112 R113 I114 T115 E118 A119 P137 T146 P150 K155 F175 G185
 L189 N197 R198 V208 H209 I225 G229 P234 S237 R245 S261 S262 G263

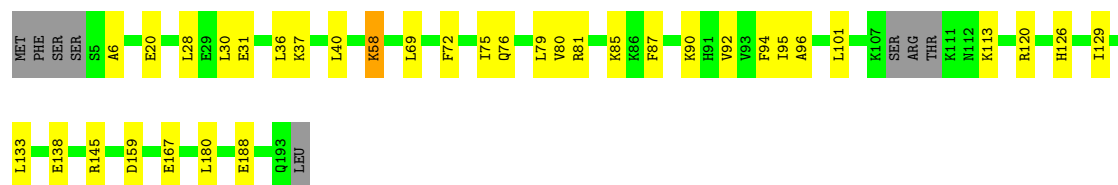
• Molecule 7: 40S ribosomal protein S5

Chain SF:  70% 22% 7%

MET THR GLU TRP GLU THR ALA ALA PRO PRO VAL VAL ALA GLU THR PRO D16 V28 Q29 I30 L35 Q36 K44 L49 G54 A58 K59 R60 F61 R62 H79 G80 R81 K85 M88 T89 V90 R91 I92 V93 L102 L103 T104 G105 E106 L109 I117 P121
 R122 E123 D124 S125 T126 R127 I128 G129 G132 T133 V134 R135 R136 D140 A150 L153 L154 R159 N165 I166 D175 I178 L196 K201 S202 N203 R204

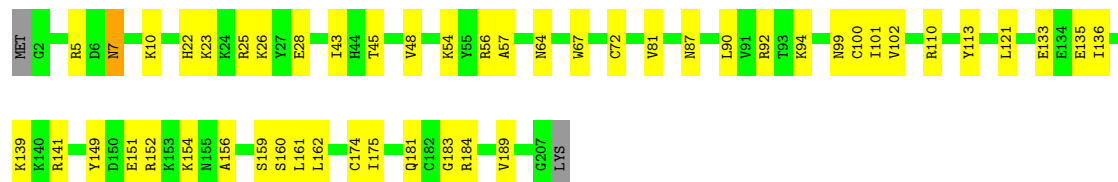
• Molecule 8: 40S ribosomal protein S7

Chain SH:  78% 18% 4%



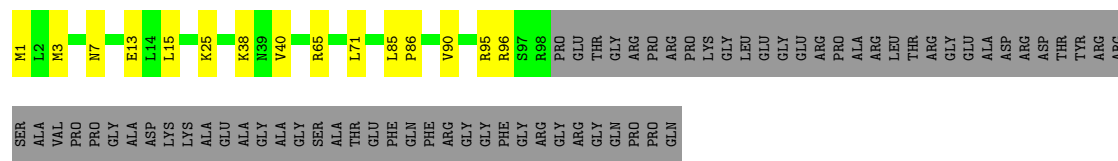
- Molecule 9: 40S ribosomal protein S8

Chain SI: 75% 23%



- Molecule 10: 40S ribosomal protein S10

Chain SK: 50% 9% 41%



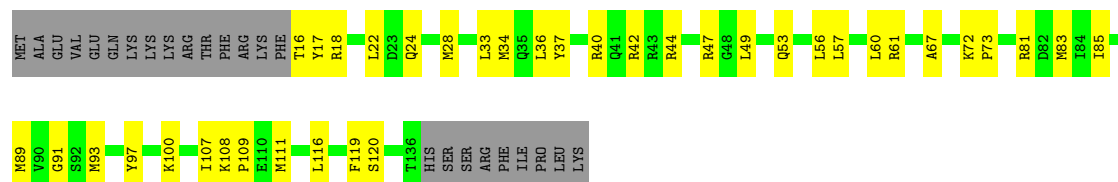
- Molecule 11: 40S ribosomal protein S11

Chain SL: 80% 16%



- Molecule 12: 40S ribosomal protein S15

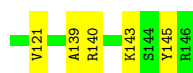
Chain SP: 57% 26% 17%



- Molecule 13: 40S ribosomal protein S16

Chain SQ: 74% 24%





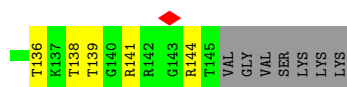
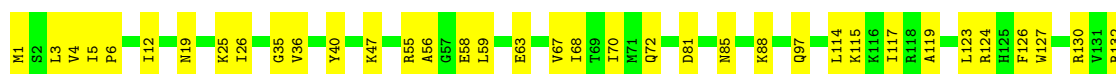
- Molecule 14: 40S ribosomal protein S17

Chain SR: 78% 20%



- Molecule 15: 40S ribosomal protein S18

Chain SS: 68% 27% 5%



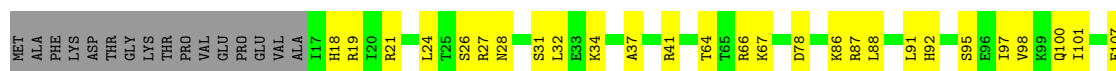
- Molecule 16: 40S ribosomal protein S19

Chain ST: 81% 18%



- Molecule 17: 40S ribosomal protein S20

Chain SU: 62% 24% 13%



- Molecule 18: 40S ribosomal protein S21

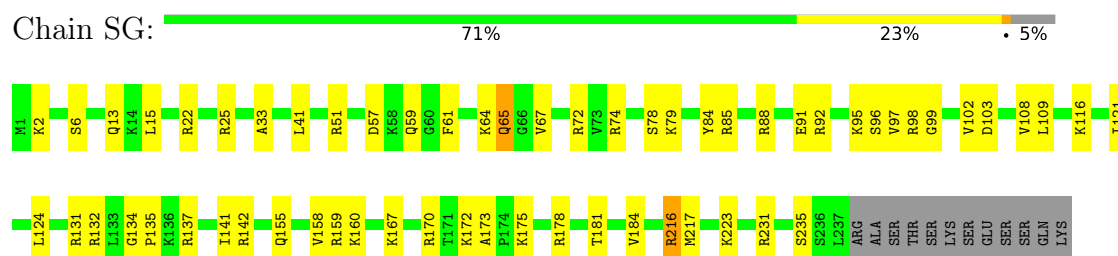
Chain SV: 77% 23%



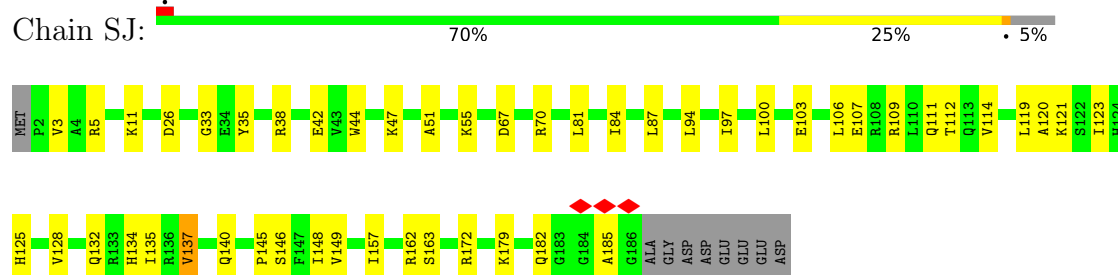
- Molecule 19: 40S ribosomal protein S23

Chain SX: 80% 18%

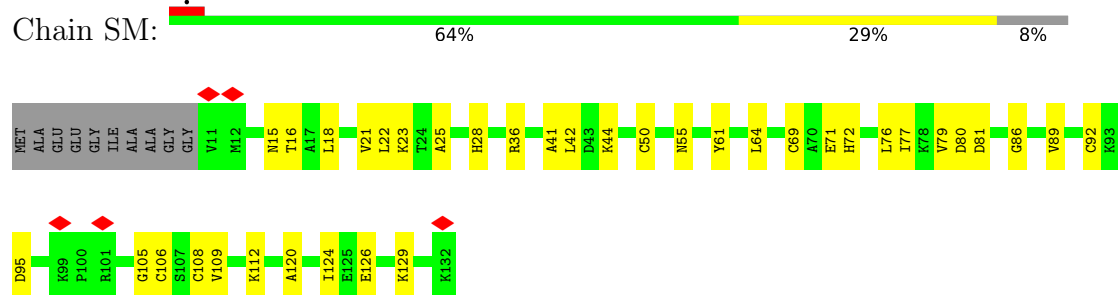
- Molecule 25: 40S ribosomal protein S6



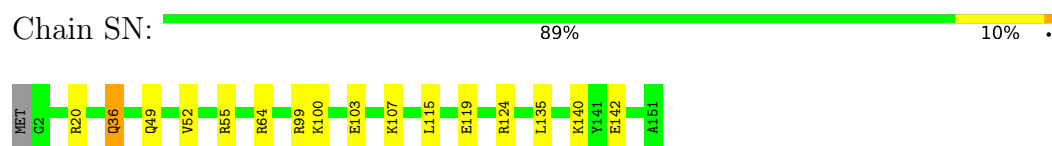
- Molecule 26: 40S ribosomal protein S9



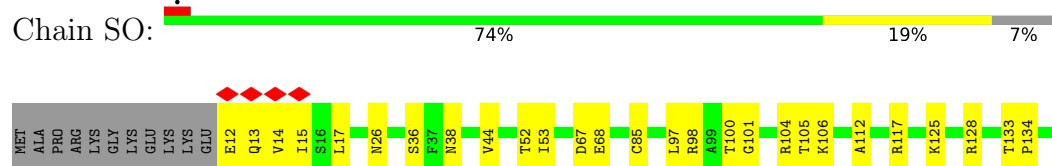
- Molecule 27: 40S ribosomal protein S12



- Molecule 28: 40S ribosomal protein S13

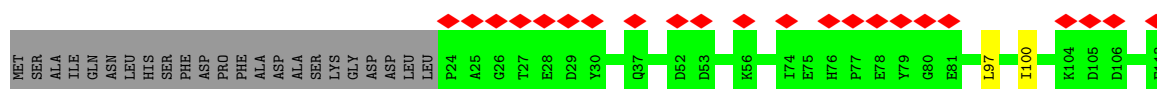
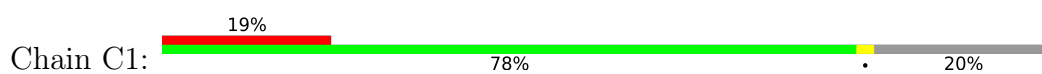


- Molecule 29: 40S ribosomal protein S14

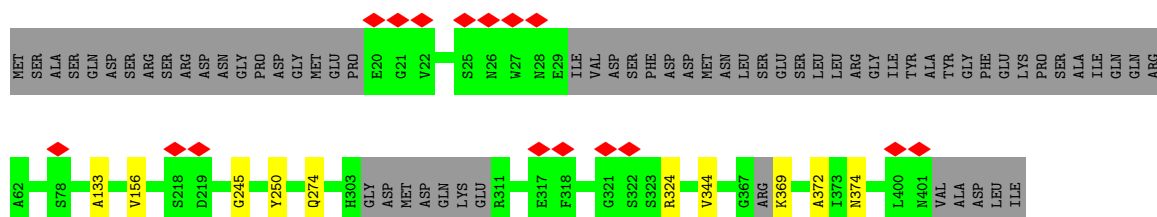
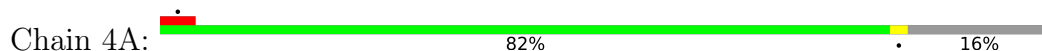


- Molecule 30: 40S ribosomal protein S15a

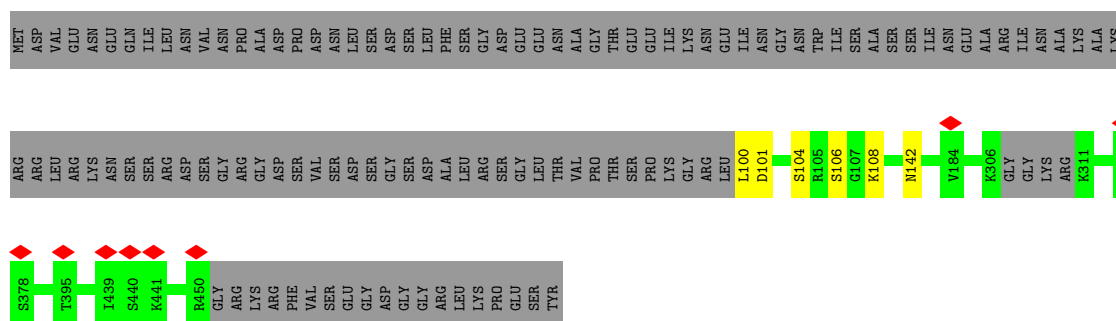
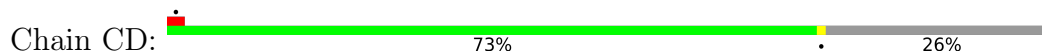




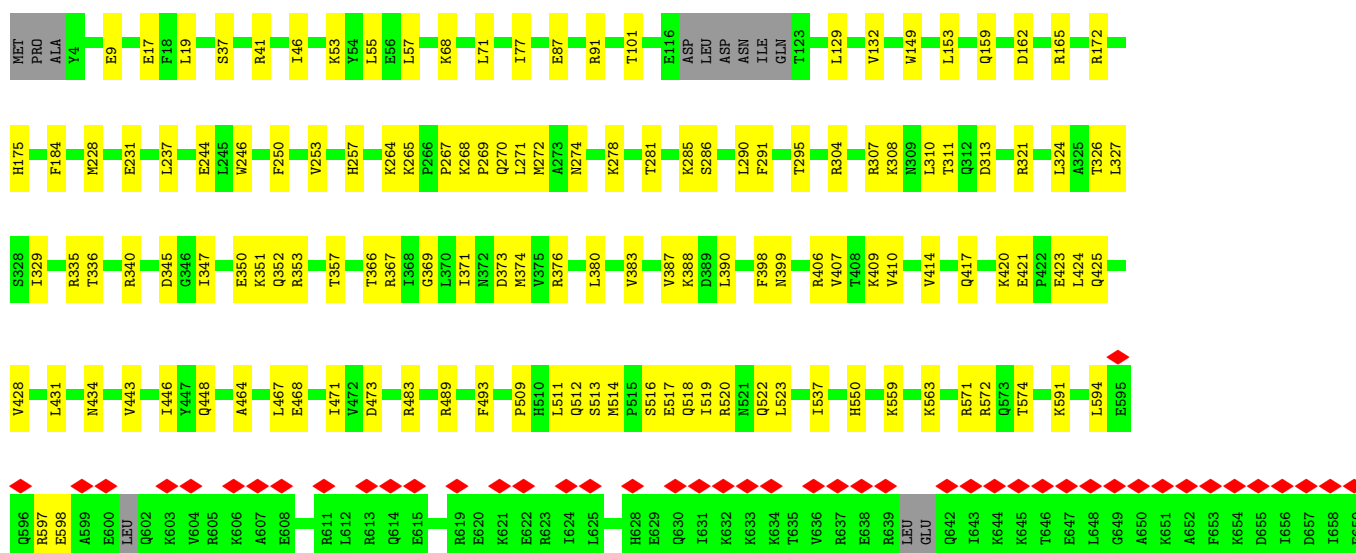
• Molecule 37: Eukaryotic initiation factor 4A-I



• Molecule 38: Programmed cell death protein 4



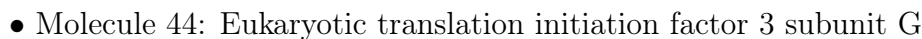
• Molecule 39: Eukaryotic translation initiation factor 3 subunit A



Response	Percentage
Yes, I have used a mobile app to book a flight	71%
No, I have not used a mobile app to book a flight	23%
I am unsure	7%

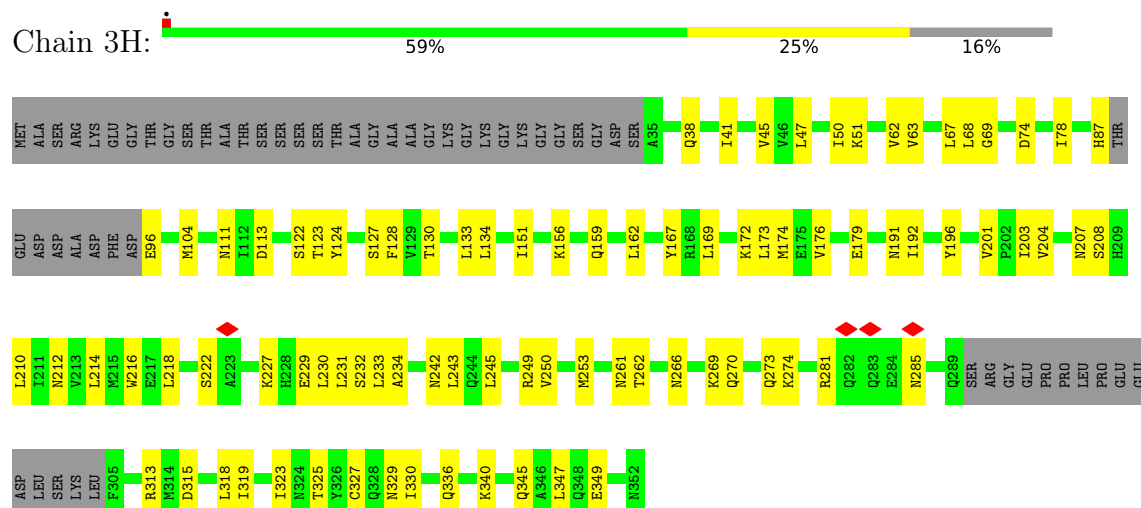


Frequency	Percentage
Daily	55%
Weekly	20%
Monthly	25%

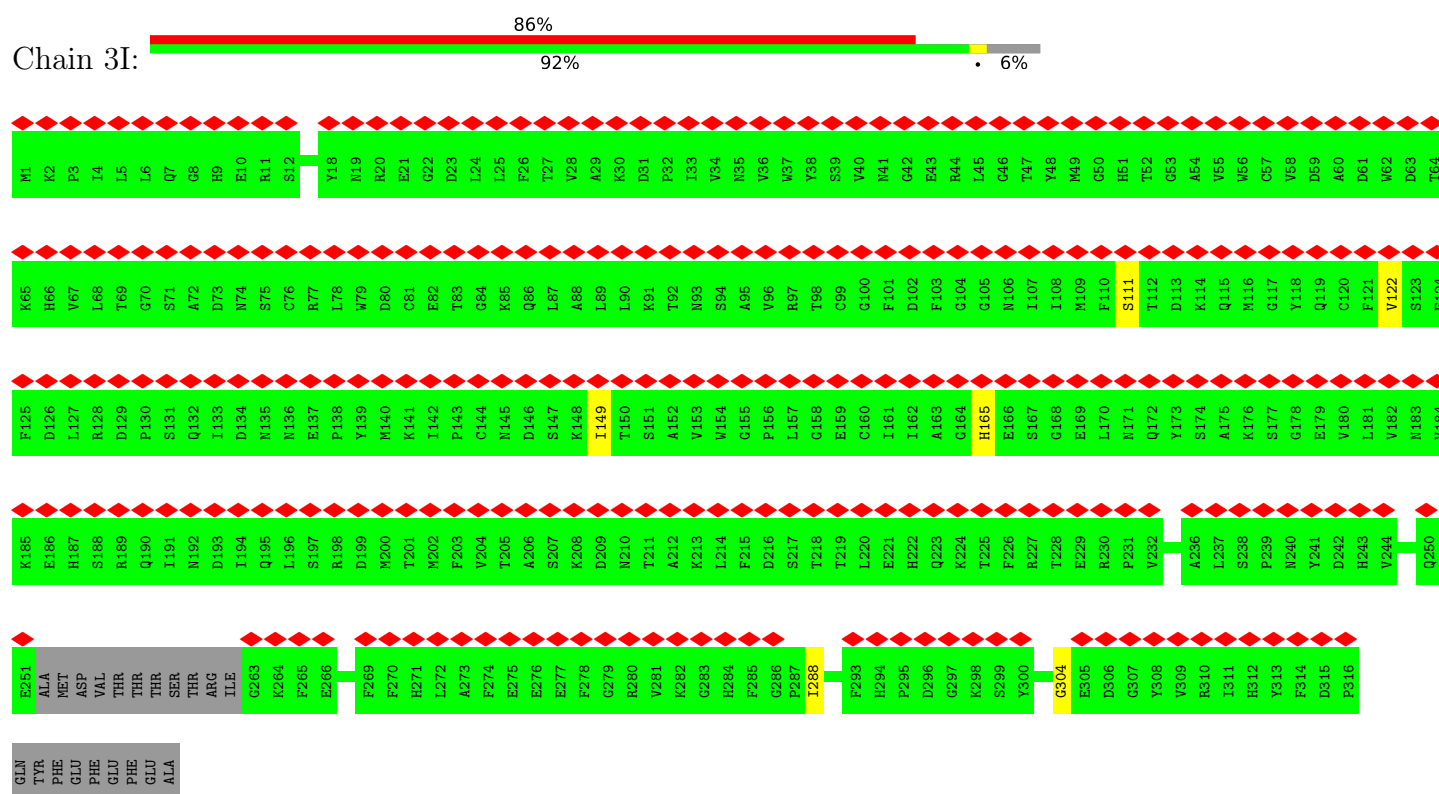


Response	Percentage
Yes, the U.S. is a democracy	20%
No, the U.S. is not a democracy	7%
Don't know	74%

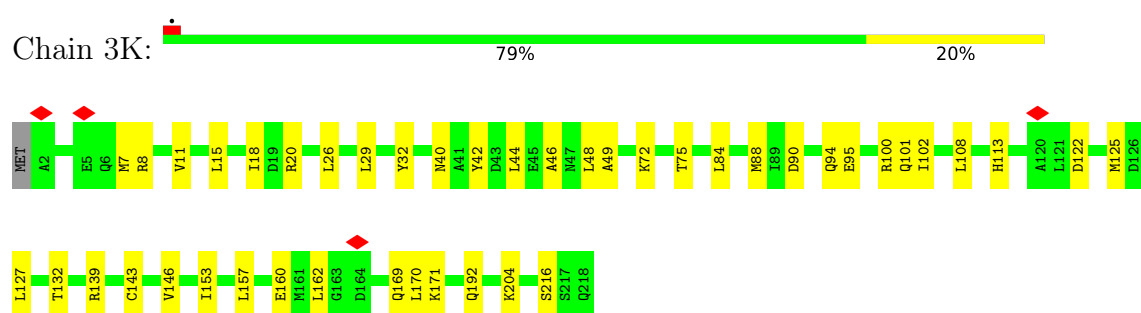




• Molecule 46: Eukaryotic translation initiation factor 3 subunit I



• Molecule 47: Eukaryotic translation initiation factor 3 subunit K



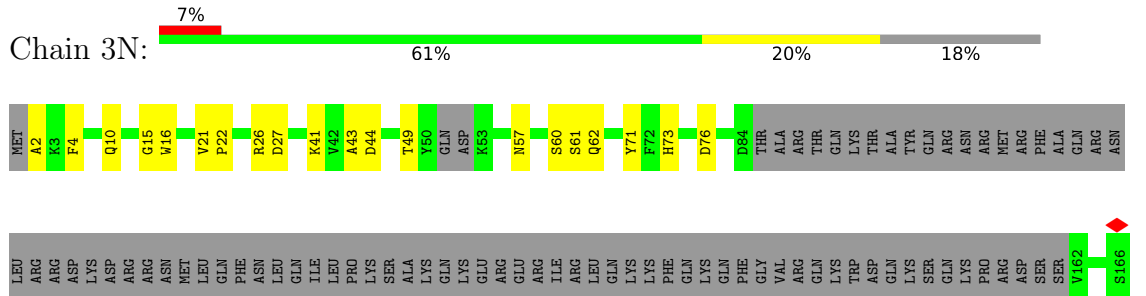
Chain 3L:



Chain 3M:



Chain 3N:





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	12788	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	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	0.375	Depositor
Minimum map value	-0.228	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	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 [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	0.44	0/294
2	S2	0.30	0/40840	0.41	1/63635 (0.0%)
3	SA	0.35	0/1778	0.66	0/2416
4	SB	0.32	0/1765	0.75	3/2362 (0.1%)
5	SD	0.35	0/1793	0.76	1/2414 (0.0%)
6	SE	0.31	0/2118	0.67	2/2849 (0.1%)
7	SF	0.32	0/1516	0.80	2/2037 (0.1%)
8	SH	0.32	0/1519	0.78	5/2033 (0.2%)
9	SI	0.32	0/1715	0.79	0/2287
10	SK	0.29	0/851	0.67	0/1147
11	SL	0.31	0/1268	0.58	0/1696
12	SP	0.31	0/1003	0.85	0/1342
13	SQ	0.33	0/1160	0.78	2/1553 (0.1%)
14	SR	0.30	0/1105	0.79	2/1484 (0.1%)
15	SS	0.26	0/1216	0.62	0/1628
16	ST	0.31	0/1131	0.69	0/1515
17	SU	0.32	0/827	0.68	0/1110
18	SV	0.31	0/643	0.64	0/860
19	SX	0.37	0/1116	0.68	0/1490
20	Sa	0.36	0/836	0.73	0/1121
21	Sc	0.33	0/508	0.79	0/680
22	Sd	0.35	0/470	0.81	0/623
23	Sg	0.24	0/2493	0.67	2/3394 (0.1%)
24	SC	0.36	0/1762	0.71	2/2381 (0.1%)
25	SG	0.25	0/1946	0.65	2/2590 (0.1%)
26	SJ	0.34	0/1550	0.65	0/2069
27	SM	0.28	0/950	0.80	0/1275
28	SN	0.29	0/1232	0.60	0/1656
29	SO	0.40	0/1062	0.74	0/1425
30	SW	0.36	0/1051	0.58	0/1406
31	SY	0.29	0/1083	0.77	1/1438 (0.1%)
32	SZ	0.29	0/604	0.78	0/810

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Sb	0.32	0/665	0.69	0/891
34	Se	0.26	0/465	0.57	0/612
35	Sf	0.22	0/560	0.68	0/745
36	C1	0.25	0/442	0.65	0/611
37	4A	0.23	0/1687	0.69	0/2344
38	CD	0.38	0/1846	0.76	1/2550 (0.0%)
39	3A	0.22	0/5463	0.60	2/7394 (0.0%)
40	3B	0.20	0/2981	0.49	1/4115 (0.0%)
41	3C	0.25	0/5154	0.67	1/6942 (0.0%)
42	3E	0.22	0/3503	0.64	3/4728 (0.1%)
43	3F	0.22	0/2126	0.61	0/2890
44	3G	0.25	0/680	0.60	0/916
45	3H	0.21	0/2458	0.58	0/3313
46	3I	0.13	0/1495	0.38	0/2073
47	3K	0.19	0/1785	0.54	0/2414
48	3L	0.24	0/3187	0.66	6/4299 (0.1%)
49	3M	0.22	0/2743	0.60	1/3697 (0.0%)
50	3N	0.21	0/3699	0.58	2/5001 (0.0%)
All	All	0.29	0/120081	0.58	42/170555 (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	2
9	SI	0	1
14	SR	0	1
19	SX	0	5
21	Sc	0	1
26	SJ	0	1
32	SZ	0	1
33	Sb	0	2
43	3F	0	1
45	3H	0	1
48	3L	0	2
All	All	0	18

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	SF	54	GLY	N-CA-C	7.70	121.44	112.50
48	3L	379	PRO	CA-C-N	7.44	135.09	121.70
48	3L	379	PRO	C-N-CA	7.44	135.09	121.70
48	3L	400	ARG	CA-C-N	-7.28	110.17	122.11
48	3L	400	ARG	C-N-CA	-7.28	110.17	122.11
23	Sg	124	SER	CA-C-N	7.16	132.05	120.60
23	Sg	124	SER	C-N-CA	7.16	132.05	120.60
49	3M	114	ASP	CA-C-O	-7.00	110.49	120.51
5	SD	36	GLY	N-CA-C	6.96	120.35	111.09
31	SY	96	LEU	N-CA-C	-6.84	105.87	114.56
24	SC	63	VAL	CA-C-N	6.82	134.56	121.54
24	SC	63	VAL	C-N-CA	6.82	134.56	121.54
8	SH	188	GLU	CA-C-N	6.62	133.85	122.06
8	SH	188	GLU	C-N-CA	6.62	133.85	122.06
7	SF	79	HIS	N-CA-C	6.38	118.38	110.91
25	SG	216	ARG	CA-C-N	6.37	133.70	121.54
25	SG	216	ARG	C-N-CA	6.37	133.70	121.54
39	3A	666	PRO	N-CA-CB	5.99	110.15	103.44
39	3A	708	PRO	N-CA-CB	5.94	110.09	103.44
4	SB	150	ILE	CA-C-N	5.92	132.85	121.54
4	SB	150	ILE	C-N-CA	5.92	132.85	121.54
14	SR	116	ASN	CB-CA-C	-5.86	109.83	116.63
13	SQ	50	LYS	N-CA-C	-5.86	106.05	113.43
14	SR	68	GLY	N-CA-C	-5.71	99.65	113.18
40	3B	507	ARG	CG-CD-NE	5.71	124.56	112.00
8	SH	20	GLU	N-CA-C	-5.66	104.95	113.89
48	3L	348	SER	CA-C-N	5.61	131.80	121.70
48	3L	348	SER	C-N-CA	5.61	131.80	121.70
8	SH	167	GLU	N-CA-C	-5.56	107.75	114.75
2	S2	1331	C	C2'-C3'-O3'	5.52	117.78	109.50
38	CD	104	SER	N-CA-C	5.49	118.54	110.59
6	SE	87	MET	CA-C-N	-5.47	113.25	123.05
6	SE	87	MET	C-N-CA	-5.47	113.25	123.05
8	SH	58	LYS	CB-CG-CD	5.31	123.50	111.30
13	SQ	107	GLU	N-CA-CB	5.24	117.91	110.16
42	3E	314	GLU	CA-CB-CG	5.22	124.55	114.10
4	SB	151	ARG	N-CA-CB	5.14	119.17	110.49
42	3E	48	THR	CA-C-N	5.12	129.67	122.46
42	3E	48	THR	C-N-CA	5.12	129.67	122.46
41	3C	407	GLU	N-CA-CB	5.11	118.72	110.40
50	3N	181	LYS	CA-C-N	-5.03	110.70	121.45
50	3N	181	LYS	C-N-CA	-5.03	110.70	121.45

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
43	3F	194	ALA	Peptide
45	3H	196	TYR	Peptide
48	3L	401	MET	Peptide
48	3L	432	HIS	Peptide
7	SF	133	THR	Peptide
7	SF	79	HIS	Peptide
9	SI	159	SER	Peptide
26	SJ	137	VAL	Peptide
14	SR	67	ARG	Peptide
19	SX	119	ARG	Sidechain
19	SX	124	LYS	Peptide
19	SX	125	VAL	Peptide
19	SX	126	ALA	Peptide
19	SX	86	PRO	Peptide
32	SZ	46	ASN	Peptide
33	Sb	33	MET	Peptide
33	Sb	82	LYS	Peptide
21	Sc	29	GLN	Peptide

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	7	0
2	S2	36535	0	18416	345	0
3	SA	1741	0	1746	34	0
4	SB	1738	0	1809	25	0
5	SD	1765	0	1865	26	0
6	SE	2076	0	2177	23	0
7	SF	1495	0	1549	28	0
8	SH	1497	0	1590	18	0
9	SI	1686	0	1772	40	0
10	SK	827	0	854	10	0
11	SL	1247	0	1323	20	0
12	SP	985	0	1031	29	0
13	SQ	1142	0	1213	25	0
14	SR	1090	0	1149	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	SS	1198	0	1261	30	0
16	ST	1112	0	1146	19	0
17	SU	817	0	882	18	0
18	SV	636	0	637	14	0
19	SX	1098	0	1167	15	0
20	Sa	821	0	870	16	0
21	Sc	506	0	536	11	0
22	Sd	459	0	448	11	0
23	Sg	2436	0	2393	53	0
24	SC	1725	0	1813	27	0
25	SG	1923	0	2088	41	0
26	SJ	1525	0	1640	36	0
27	SM	940	0	965	26	0
28	SN	1208	0	1294	14	0
29	SO	1049	0	1073	18	0
30	SW	1034	0	1080	16	0
31	SY	1065	0	1142	35	0
32	SZ	598	0	656	15	0
33	Sb	651	0	672	13	0
34	Se	459	0	503	8	0
35	Sf	548	0	555	11	0
36	C1	443	0	201	2	0
37	4A	1691	0	753	5	0
38	CD	1841	0	998	5	0
39	3A	5379	0	5155	92	0
40	3B	2966	0	1764	19	0
41	3C	5070	0	5110	98	0
42	3E	3437	0	3433	70	0
43	3F	2090	0	2092	57	0
44	3G	667	0	647	14	0
45	3H	2413	0	2411	70	0
46	3I	1497	0	676	3	0
47	3K	1750	0	1717	30	0
48	3L	3111	0	3085	61	0
49	3M	2705	0	2759	55	0
50	3N	3617	0	3495	73	0
51	S2	22	0	0	0	0
51	SG	1	0	0	0	0
52	Sa	1	0	0	0	0
52	Sd	1	0	0	0	0
52	Sf	1	0	0	0	0
All	All	114565	0	93887	1511	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 7.

All (1511) 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)
41:3C:697:TYR:HH	41:3C:708:ARG:N	1.57	1.03
2:S2:886:A:N6	2:S2:901:G:C4	2.31	0.98
2:S2:885:U:H3	2:S2:901:G:H1	1.07	0.96
20:Sa:88:SER:O	20:Sa:92:ARG:HB2	1.64	0.96
2:S2:1609:C:H42	2:S2:1630:A:H61	1.02	0.93
42:3E:99:GLU:O	42:3E:103:GLN:HB2	1.66	0.93
2:S2:1752:C:C4	2:S2:1779:G:N2	2.38	0.91
9:SI:99:ASN:HA	9:SI:175:ILE:O	1.71	0.91
39:3A:518:GLN:O	39:3A:522:GLN:HB2	1.71	0.90
2:S2:1548:G:C6	2:S2:1586:U:O4	2.28	0.87
38:CD:100:LEU:HD12	38:CD:101:ASP:N	1.92	0.84
23:Sg:30:MET:HA	23:Sg:43:TRP:O	1.77	0.84
48:3L:401:MET:HB2	48:3L:408:VAL:HG22	1.60	0.83
2:S2:533:A:H61	2:S2:550:C:N4	1.77	0.83
7:SF:127:ARG:HG3	7:SF:129:GLY:H	1.44	0.83
43:3F:331:ILE:O	43:3F:335:LEU:HB2	1.81	0.81
50:3N:252:LEU:O	50:3N:256:MET:HB2	1.81	0.80
11:SL:18:GLN:HA	11:SL:18:GLN:HE21	1.44	0.80
15:SS:115:LYS:HD3	15:SS:126:PHE:HB2	1.62	0.80
3:SA:209:GLU:O	3:SA:213:GLU:HB2	1.82	0.79
2:S2:1755:C:N4	2:S2:1756:C:N4	2.31	0.78
2:S2:1115:U:C2	2:S2:1118:C:N4	2.51	0.78
7:SF:134:VAL:HG13	7:SF:135:ARG:HG2	1.65	0.78
2:S2:886:A:N6	2:S2:901:G:C5	2.53	0.76
2:S2:1755:C:C4	2:S2:1756:C:N4	2.54	0.76
2:S2:1115:U:N3	2:S2:1118:C:N4	2.33	0.76
2:S2:323:C:H2'	2:S2:327:G:H22	1.51	0.76
2:S2:1609:C:N4	2:S2:1630:A:H61	1.83	0.76
2:S2:533:A:N6	2:S2:550:C:N4	2.33	0.75
44:3G:257:GLU:HG3	44:3G:260:ARG:HH22	1.50	0.75
10:SK:7:ASN:HD22	10:SK:40:VAL:HG12	1.52	0.75
50:3N:359:ARG:HB3	50:3N:375:CYS:HB2	1.67	0.75
41:3C:862:LYS:HD2	45:3H:250:VAL:HG11	1.68	0.74
9:SI:152:ARG:O	9:SI:156:ALA:HB2	1.88	0.73
2:S2:384:U:O4	9:SI:5:ARG:NH2	2.23	0.72
13:SQ:53:GLU:O	13:SQ:57:LEU:HB3	1.89	0.72
2:S2:1752:C:N3	2:S2:1779:G:N1	2.36	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:3N:169:GLU:HB2	50:3N:521:SER:HB2	1.72	0.72
2:S2:1609:C:H42	2:S2:1630:A:N6	1.83	0.71
2:S2:1752:C:C2	2:S2:1779:G:N1	2.57	0.71
2:S2:1752:C:N3	2:S2:1779:G:C2	2.58	0.71
27:SM:41:ALA:O	27:SM:44:LYS:C	2.34	0.71
9:SI:67:TRP:HE1	9:SI:162:LEU:HD21	1.54	0.71
15:SS:12:ILE:HD12	15:SS:19:ASN:HD21	1.56	0.71
12:SP:83:MET:HB3	12:SP:116:LEU:HD13	1.72	0.70
2:S2:570:C:H4'	31:SY:36:PRO:HG3	1.73	0.70
2:S2:952:G:H21	29:SO:52:THR:HG21	1.57	0.70
2:S2:57:U:O2	2:S2:500:A:N7	2.25	0.69
16:ST:85:ASN:HB2	16:ST:88:MET:HB2	1.73	0.69
2:S2:748:C:H42	2:S2:795:A:N6	1.89	0.69
21:Sc:13:ARG:HH22	50:3N:423:THR:HA	1.58	0.69
50:3N:73:HIS:HB3	50:3N:76:ASP:HB3	1.73	0.69
7:SF:140:ASP:HB2	21:Sc:46:VAL:HG12	1.73	0.69
1:Ln:8:LYS:NZ	2:S2:1846:G:O6	2.26	0.69
39:3A:513:SER:OG	39:3A:517:GLU:OE2	2.10	0.68
39:3A:446:ILE:HD12	39:3A:512:GLN:HE21	1.59	0.68
2:S2:1755:C:N4	2:S2:1756:C:H41	1.92	0.68
33:Sb:36:LYS:H	33:Sb:78:SER:HB3	1.58	0.68
50:3N:194:GLU:HB2	50:3N:360:TYR:HB2	1.74	0.68
2:S2:1609:C:N3	2:S2:1630:A:N1	2.41	0.68
23:Sg:87:LEU:HD11	23:Sg:111:VAL:HG11	1.74	0.68
39:3A:270:GLN:HE21	39:3A:274:ASN:HD22	1.42	0.68
41:3C:140:THR:OG1	41:3C:144:LYS:NZ	2.27	0.67
43:3F:345:GLN:OE1	48:3L:537:ARG:NH1	2.27	0.67
40:3B:565:ILE:HA	40:3B:581:HIS:HA	1.77	0.67
49:3M:156:LEU:HB2	49:3M:161:LYS:HE2	1.74	0.67
5:SD:59:LEU:HD11	44:3G:308:LEU:HD11	1.76	0.67
33:Sb:37:CYS:HA	33:Sb:77:CYS:HB3	1.76	0.66
2:S2:748:C:N4	2:S2:795:A:N6	2.42	0.66
27:SM:22:LEU:HD21	27:SM:89:VAL:HA	1.78	0.66
49:3M:196:ASN:HB2	49:3M:199:GLN:HE21	1.59	0.66
50:3N:357:ALA:HB3	50:3N:377:HIS:HB2	1.77	0.66
36:C1:97:LEU:O	36:C1:100:ILE:O	2.14	0.66
2:S2:506:G:OP1	31:SY:108:LYS:NZ	2.28	0.65
8:SH:95:ILE:HD11	8:SH:133:LEU:HD13	1.78	0.65
27:SM:41:ALA:O	27:SM:44:LYS:O	2.14	0.65
50:3N:22:PRO:O	50:3N:26:ARG:NH1	2.30	0.65
35:Sf:107:LYS:HG2	35:Sf:117:LEU:HD21	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:3H:130:THR:H	45:3H:133:LEU:HB2	1.62	0.64
50:3N:179:LEU:HA	50:3N:182:MET:HE1	1.79	0.64
2:S2:1017:U:H5'	28:SN:55:ARG:HE	1.62	0.64
9:SI:113:TYR:HD2	9:SI:121:LEU:HD22	1.61	0.64
7:SF:29:GLN:HG3	50:3N:475:GLU:HG3	1.79	0.64
45:3H:62:VAL:HA	45:3H:122:SER:O	1.97	0.64
3:SA:53:ARG:HG2	18:SV:83:PHE:HD2	1.63	0.64
15:SS:141:ARG:HA	15:SS:144:ARG:HB2	1.77	0.64
2:S2:1488:C:O2'	2:S2:1490:G:OP2	2.16	0.63
26:SJ:114:VAL:HG21	26:SJ:135:ILE:HD13	1.81	0.63
31:SY:130:LYS:HG3	31:SY:131:PRO:HD3	1.81	0.63
44:3G:300:VAL:HG13	44:3G:312:VAL:HG21	1.81	0.63
50:3N:21:VAL:HG12	50:3N:26:ARG:HH12	1.63	0.63
2:S2:1138:C:O2'	18:SV:61:ARG:NH1	2.31	0.63
4:SB:68:GLU:HA	4:SB:84:PHE:O	1.98	0.63
8:SH:58:LYS:HB2	8:SH:90:LYS:HG2	1.80	0.63
37:4A:250:TYR:HA	37:4A:374:ASN:O	1.98	0.63
40:3B:342:TRP:HA	40:3B:349:LEU:HA	1.80	0.63
2:S2:1752:C:C4	2:S2:1779:G:C2	2.86	0.63
43:3F:211:MET:HE1	45:3H:214:LEU:HD13	1.81	0.63
2:S2:1562:C:H2'	2:S2:1563:G:H8	1.64	0.63
49:3M:224:LEU:HD11	49:3M:245:VAL:HG11	1.81	0.63
2:S2:533:A:N6	2:S2:550:C:H42	1.93	0.63
2:S2:990:A:OP2	20:Sa:37:LYS:NZ	2.31	0.63
4:SB:198:GLU:HB2	4:SB:210:VAL:HG21	1.80	0.63
23:Sg:176:VAL:HB	23:Sg:186:THR:HB	1.79	0.63
43:3F:302:ASN:OD1	43:3F:306:ARG:NH1	2.32	0.63
11:SL:42:LEU:HD13	11:SL:72:ILE:HD11	1.81	0.62
23:Sg:145:GLU:O	23:Sg:175:LYS:NZ	2.32	0.62
2:S2:24:C:OP1	26:SJ:11:LYS:NZ	2.27	0.62
2:S2:1658:G:OP2	2:S2:1660:C:N4	2.32	0.62
9:SI:100:CYS:O	9:SI:174:CYS:HA	1.99	0.62
3:SA:91:ALA:O	3:SA:94:THR:O	2.16	0.62
5:SD:137:VAL:HG22	5:SD:151:LYS:HG2	1.81	0.62
3:SA:200:ASP:HA	3:SA:203:PHE:HD2	1.63	0.62
14:SR:111:PHE:HB3	14:SR:114:LEU:HD21	1.79	0.62
40:3B:505:ARG:HE	40:3B:554:VAL:HB	1.65	0.62
39:3A:321:ARG:HD2	39:3A:423:GLU:HG3	1.82	0.62
41:3C:633:LEU:HA	41:3C:636:ILE:HG22	1.80	0.62
41:3C:855:LEU:HD13	45:3H:243:LEU:HD22	1.81	0.62
2:S2:1543:U:OP1	13:SQ:37:ARG:NH2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:3F:218:SER:HB3	43:3F:220:LEU:HD23	1.82	0.62
31:SY:82:ALA:O	31:SY:86:GLU:HB3	1.99	0.62
2:S2:1005:G:OP2	4:SB:162:ARG:NH2	2.33	0.62
2:S2:1548:G:O6	2:S2:1586:U:C4	2.53	0.62
6:SE:11:ARG:NH1	6:SE:24:THR:OG1	2.33	0.62
39:3A:175:HIS:HD2	39:3A:228:MET:HE2	1.64	0.62
43:3F:264:GLY:HA2	45:3H:204:VAL:HA	1.82	0.62
18:SV:35:ASN:OD1	24:SC:267:GLN:NE2	2.33	0.61
49:3M:80:GLU:HB3	49:3M:119:VAL:HG21	1.81	0.61
2:S2:1569:A:OP2	16:ST:97:LYS:NZ	2.33	0.61
3:SA:207:PRO:HA	3:SA:210:ILE:HB	1.82	0.61
2:S2:529:A:N6	2:S2:557:U:H3	1.99	0.61
43:3F:261:ARG:HE	45:3H:208:SER:HA	1.66	0.61
2:S2:380:G:OP2	9:SI:181:GLN:NE2	2.33	0.61
6:SE:185:GLY:H	6:SE:189:LEU:HD13	1.66	0.61
15:SS:85:ASN:OD1	15:SS:97:GLN:NE2	2.34	0.61
41:3C:507:ILE:O	41:3C:511:TYR:HB3	1.99	0.61
41:3C:659:ASN:OD1	41:3C:662:GLN:NE2	2.34	0.61
43:3F:332:ASN:ND2	48:3L:522:TYR:OH	2.34	0.61
2:S2:1759:G:N2	2:S2:1773:C:OP1	2.33	0.61
9:SI:101:ILE:HD13	9:SI:174:CYS:HB3	1.83	0.61
9:SI:7:ASN:C	9:SI:7:ASN:HD22	2.09	0.60
3:SA:38:ILE:HD11	3:SA:47:TYR:HB3	1.83	0.60
23:Sg:272:GLN:NE2	23:Sg:284:PRO:O	2.34	0.60
44:3G:267:ARG:HB2	44:3G:286:SER:HB3	1.83	0.60
6:SE:19:MET:SD	6:SE:51:ARG:NH2	2.74	0.60
49:3M:117:THR:HG23	49:3M:120:ARG:H	1.66	0.60
19:SX:68:LYS:HB3	19:SX:91:LEU:HD22	1.83	0.60
42:3E:353:ILE:HD11	42:3E:391:VAL:HG23	1.82	0.60
2:S2:925:G:H1	2:S2:1017:U:H3	0.81	0.60
2:S2:1160:U:O4	19:SX:2:GLY:N	2.34	0.60
2:S2:1331:C:O2'	2:S2:1332:A:OP2	2.06	0.60
45:3H:47:LEU:HD13	45:3H:50:ILE:HD11	1.84	0.60
45:3H:68:LEU:HD11	45:3H:104:MET:HE1	1.84	0.60
2:S2:1781:A:O2'	2:S2:1782:G:N7	2.31	0.60
3:SA:40:LYS:NZ	14:SR:101:ASP:OD2	2.34	0.60
26:SJ:112:THR:HG22	26:SJ:123:ILE:HD11	1.84	0.60
2:S2:1536:G:H2'	2:S2:1537:A:H8	1.66	0.60
26:SJ:182:GLN:O	26:SJ:185:ALA:O	2.19	0.60
31:SY:82:ALA:O	31:SY:86:GLU:CB	2.50	0.60
43:3F:184:VAL:HG12	43:3F:232:PHE:HE1	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:3N:222:ARG:HG3	50:3N:325:GLN:HG3	1.83	0.60
2:S2:919:A:OP2	28:SN:64:ARG:NH2	2.32	0.59
9:SI:57:ALA:HB2	9:SI:183:GLY:HA2	1.84	0.59
41:3C:637:GLN:HE22	41:3C:683:GLU:HA	1.65	0.59
8:SH:101:LEU:HD13	8:SH:120:ARG:HG2	1.84	0.59
33:Sb:83:GLN:NE2	33:Sb:84:HIS:O	2.34	0.59
48:3L:341:LEU:HD12	48:3L:343:ILE:H	1.66	0.59
23:Sg:152:SER:H	23:Sg:169:GLY:HA2	1.67	0.59
29:SO:44:VAL:HG13	29:SO:53:ILE:HB	1.85	0.59
50:3N:244:ASN:HD21	50:3N:369:ILE:HA	1.66	0.59
15:SS:25:LYS:HD2	15:SS:55:ARG:HD3	1.83	0.59
39:3A:172:ARG:HA	39:3A:228:MET:HE1	1.83	0.59
43:3F:283:LEU:HA	43:3F:286:VAL:HG12	1.83	0.59
2:S2:860:G:H21	30:SW:107:SER:HB2	1.67	0.59
39:3A:443:VAL:HG12	39:3A:493:PHE:HE2	1.67	0.59
49:3M:121:TYR:HE1	49:3M:164:LEU:HB2	1.68	0.59
23:Sg:236:ILE:HD13	23:Sg:252:THR:HB	1.85	0.59
45:3H:38:GLN:HA	45:3H:201:VAL:HB	1.85	0.59
2:S2:1274:G:OP1	10:SK:1:MET:N	2.34	0.59
6:SE:197:ASN:HB3	6:SE:209:HIS:HB2	1.84	0.59
7:SF:102:LEU:HD23	32:SZ:67:LEU:HD23	1.84	0.59
41:3C:641:ARG:HH21	50:3N:49:THR:HG23	1.67	0.59
43:3F:323:PHE:HZ	45:3H:345:GLN:HA	1.68	0.59
5:SD:42:THR:HG23	5:SD:45:ARG:H	1.67	0.59
33:Sb:40:CYS:SG	33:Sb:41:TYR:N	2.72	0.59
48:3L:480:ASP:HB3	48:3L:486:PHE:HB3	1.83	0.59
7:SF:59:LYS:HB2	7:SF:62:ARG:HE	1.68	0.58
45:3H:242:ASN:HA	45:3H:245:LEU:HD12	1.85	0.58
15:SS:141:ARG:O	15:SS:144:ARG:C	2.45	0.58
23:Sg:219:TRP:HA	23:Sg:227:LEU:HB2	1.84	0.58
24:SC:104:ASP:HB3	24:SC:130:ILE:HG13	1.85	0.58
39:3A:373:ASP:HA	39:3A:376:ARG:HG2	1.85	0.58
45:3H:38:GLN:NE2	45:3H:74:ASP:O	2.35	0.58
2:S2:71:G:O6	25:SG:170:ARG:NH2	2.37	0.58
2:S2:528:A:H2'	2:S2:529:A:H8	1.67	0.58
2:S2:1744:G:O2'	2:S2:1789:G:N2	2.35	0.58
23:Sg:192:THR:OG1	23:Sg:213:ASP:OD2	2.20	0.58
49:3M:327:GLN:O	49:3M:330:ARG:NH1	2.36	0.58
2:S2:394:G:H5'	11:SL:81:LYS:HD3	1.85	0.58
2:S2:1358:U:OP2	24:SC:123:ARG:NH2	2.36	0.58
7:SF:35:LEU:HG	7:SF:117:ILE:HG13	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:SK:13:GLU:OE2	10:SK:38:LYS:NZ	2.36	0.58
23:Sg:206:LEU:HD21	23:Sg:218:LEU:HB2	1.85	0.58
48:3L:470:MET:HB2	48:3L:474:LYS:HB3	1.85	0.58
2:S2:77:A:OP2	25:SG:155:GLN:NE2	2.36	0.58
5:SD:211:VAL:O	14:SR:20:TYR:OH	2.21	0.58
27:SM:126:GLU:OE1	27:SM:129:LYS:NZ	2.37	0.58
39:3A:55:LEU:HD21	39:3A:71:LEU:HD21	1.85	0.58
39:3A:511:LEU:HD23	39:3A:512:GLN:HG3	1.86	0.58
41:3C:94:LYS:HE2	41:3C:99:LYS:HG2	1.85	0.58
2:S2:994:C:N4	20:Sa:14:GLY:O	2.35	0.58
11:SL:22:ARG:NH1	11:SL:23:VAL:O	2.36	0.58
39:3A:387:VAL:HA	39:3A:390:LEU:HD23	1.86	0.58
39:3A:572:ARG:NH1	45:3H:111:ASN:OD1	2.36	0.58
42:3E:274:LEU:HA	42:3E:277:LEU:HD12	1.84	0.58
2:S2:399:C:O4'	19:SX:11:ARG:NH1	2.35	0.58
6:SE:66:MET:SD	6:SE:78:THR:OG1	2.62	0.58
39:3A:366:THR:HG23	39:3A:369:GLY:H	1.69	0.58
49:3M:156:LEU:HD23	49:3M:160:LYS:HE2	1.86	0.58
25:SG:74:ARG:NH1	25:SG:96:SER:OG	2.37	0.58
39:3A:514:MET:HG3	39:3A:516:SER:H	1.68	0.58
2:S2:880:G:H3'	2:S2:881:G:H8	1.69	0.58
4:SB:107:ARG:NH1	29:SO:133:THR:O	2.36	0.58
5:SD:106:ARG:HD2	5:SD:173:ARG:HB3	1.86	0.58
42:3E:401:TYR:HB3	43:3F:336:MET:HE1	1.85	0.58
43:3F:212:SER:O	43:3F:214:LYS:NZ	2.34	0.58
17:SU:98:VAL:HA	17:SU:101:ILE:HB	1.86	0.57
45:3H:169:LEU:HB3	45:3H:174:MET:HE3	1.85	0.57
11:SL:75:GLY:HA3	11:SL:88:ILE:HD12	1.86	0.57
42:3E:255:ARG:HB2	42:3E:292:ILE:HD11	1.85	0.57
2:S2:129:C:H4'	2:S2:130:G:H5'	1.86	0.57
5:SD:94:ARG:NH1	38:CD:142:ASN:OD1	2.36	0.57
21:Sc:17:VAL:H	21:Sc:52:GLU:HG3	1.70	0.57
30:SW:24:GLN:NE2	30:SW:64:ASN:OD1	2.36	0.57
43:3F:97:VAL:HG12	45:3H:47:LEU:HB3	1.85	0.57
12:SP:67:ALA:HB2	12:SP:73:PRO:HG3	1.87	0.57
22:Sd:26:ASN:HD22	22:Sd:27:ARG:N	2.02	0.57
24:SC:168:GLY:N	24:SC:179:THR:O	2.34	0.57
43:3F:356:ASN:OD1	45:3H:313:ARG:NH2	2.38	0.57
2:S2:1228:A:H2'	2:S2:1229:G:C8	2.39	0.57
9:SI:87:ASN:HB3	9:SI:90:LEU:HD23	1.85	0.57
39:3A:537:ILE:HD11	43:3F:304:VAL:HG11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S2:522:A:H5''	26:SJ:145:PRO:HD2	1.85	0.57
2:S2:1374:C:O2'	2:S2:1464:C:O2	2.22	0.57
26:SJ:182:GLN:O	26:SJ:185:ALA:C	2.47	0.57
2:S2:1644:C:H4'	13:SQ:140:ARG:HB2	1.86	0.57
41:3C:480:CYS:SG	41:3C:513:LYS:NZ	2.78	0.57
50:3N:218:ARG:O	50:3N:326:GLN:NE2	2.38	0.57
2:S2:1679:A:N6	7:SF:58:ALA:O	2.38	0.57
5:SD:132:LYS:HD3	5:SD:189:MET:HE3	1.87	0.57
7:SF:28:VAL:HG21	7:SF:109:LEU:HB2	1.86	0.57
31:SY:126:GLY:HA2	31:SY:129:LYS:HB2	1.87	0.57
50:3N:245:VAL:HG12	50:3N:276:LEU:HB3	1.87	0.57
50:3N:291:VAL:HG12	50:3N:312:LEU:HD13	1.87	0.57
2:S2:1284:A:N6	2:S2:1313:A:O2'	2.38	0.57
42:3E:102:ARG:O	42:3E:105:GLN:NE2	2.38	0.57
2:S2:1756:C:O2	2:S2:1776:G:C6	2.58	0.56
15:SS:139:THR:O	15:SS:144:ARG:NH2	2.37	0.56
31:SY:10:ARG:O	31:SY:11:LYS:C	2.48	0.56
35:Sf:108:VAL:HG13	35:Sf:112:GLY:HA2	1.87	0.56
41:3C:507:ILE:HA	41:3C:510:THR:HG22	1.86	0.56
2:S2:1209:A:H5''	20:Sa:82:LYS:HE2	1.87	0.56
41:3C:613:MET:HE3	50:3N:41:LYS:H	1.70	0.56
2:S2:587:A:H5'	2:S2:592:C:H42	1.70	0.56
2:S2:1277:C:H2'	2:S2:1278:A:H8	1.70	0.56
3:SA:41:ARG:HH11	3:SA:45:GLY:HA2	1.71	0.56
19:SX:128:VAL:HG13	19:SX:138:LYS:HE3	1.88	0.56
24:SC:166:ARG:HB2	24:SC:248:TYR:HD1	1.69	0.56
31:SY:60:PHE:HA	31:SY:70:THR:O	2.05	0.56
46:3I:149:ILE:HA	46:3I:165:HIS:HA	1.87	0.56
49:3M:249:LEU:HD23	49:3M:281:THR:HG21	1.87	0.56
2:S2:1228:A:H2'	2:S2:1229:G:H8	1.69	0.56
4:SB:150:ILE:HG23	14:SR:131:PRO:HA	1.88	0.56
7:SF:125:SER:HB2	7:SF:203:ASN:HD21	1.69	0.56
23:Sg:110:SER:HB2	23:Sg:153:CYS:HA	1.88	0.56
39:3A:523:LEU:HG	45:3H:347:LEU:HD13	1.88	0.56
40:3B:478:ILE:HG22	40:3B:497:GLN:HG3	1.86	0.56
43:3F:90:ARG:HA	43:3F:235:LEU:HD22	1.87	0.56
2:S2:1566:G:H1	16:ST:97:LYS:HE2	1.70	0.56
45:3H:173:LEU:HA	45:3H:176:VAL:HG22	1.88	0.56
2:S2:1507:G:H22	35:Sf:87:THR:HA	1.69	0.56
49:3M:141:PRO:HB2	49:3M:146:GLN:HG2	1.86	0.56
50:3N:487:ALA:HA	50:3N:490:ILE:HD12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S2:919:A:O2'	2:S2:1020:A:N6	2.37	0.56
23:Sg:83:TRP:HA	23:Sg:107:ASP:HB2	1.88	0.56
40:3B:545:GLU:HA	40:3B:557:ASP:O	2.05	0.56
41:3C:486:VAL:HG13	41:3C:502:ILE:HD11	1.87	0.56
41:3C:710:ILE:O	41:3C:715:HIS:NE2	2.39	0.56
10:SK:85:LEU:HD12	10:SK:86:PRO:HD2	1.88	0.56
24:SC:178:HIS:ND1	24:SC:221:ASP:OD2	2.32	0.56
43:3F:289:TYR:OH	43:3F:300:ALA:O	2.24	0.56
44:3G:238:ASN:O	44:3G:290:ARG:NH1	2.39	0.56
2:S2:1076:G:OP2	28:SN:107:LYS:NZ	2.33	0.56
2:S2:1216:C:N4	2:S2:1342:U:OP1	2.33	0.56
2:S2:1228:A:O2'	2:S2:1634:A:N3	2.37	0.56
25:SG:59:GLN:OE1	25:SG:72:ARG:NH2	2.38	0.56
49:3M:104:GLN:NE2	49:3M:108:ASN:OD1	2.39	0.56
49:3M:258:ASN:OD1	49:3M:259:ASN:ND2	2.39	0.56
50:3N:267:ILE:HD11	50:3N:278:PHE:HB3	1.87	0.56
2:S2:94:G:HO2'	2:S2:508:A:HO2'	1.49	0.55
2:S2:748:C:N4	2:S2:795:A:H61	2.03	0.55
2:S2:750:C:H41	2:S2:793:G:H21	1.54	0.55
31:SY:54:VAL:HG22	31:SY:76:TYR:HB2	1.89	0.55
40:3B:549:MET:HA	40:3B:554:VAL:HG22	1.87	0.55
48:3L:364:ASN:HA	48:3L:367:MET:HG2	1.87	0.55
2:S2:379:C:O2	9:SI:5:ARG:NH1	2.40	0.55
2:S2:1422:G:H1'	2:S2:1424:G:C8	2.41	0.55
2:S2:1648:G:O2'	2:S2:1674:G:O6	2.23	0.55
12:SP:22:LEU:HD11	12:SP:109:PRO:HB3	1.89	0.55
2:S2:444:G:O6	9:SI:26:LYS:NZ	2.39	0.55
2:S2:677:G:OP1	28:SN:124:ARG:NH1	2.39	0.55
41:3C:759:GLU:HA	41:3C:762:ASN:HB2	1.87	0.55
48:3L:333:ILE:HB	48:3L:381:ARG:HG3	1.89	0.55
48:3L:430:ASN:H	48:3L:436:HIS:HE1	1.55	0.55
50:3N:171:LYS:HB2	50:3N:519:VAL:HG13	1.88	0.55
2:S2:1115:U:O2'	2:S2:1117:C:OP2	2.25	0.55
23:Sg:6:THR:O	23:Sg:310:TRP:HA	2.06	0.55
23:Sg:65:PHE:O	23:Sg:83:TRP:N	2.38	0.55
28:SN:49:GLN:HA	28:SN:52:VAL:HG12	1.88	0.55
39:3A:68:LYS:HD2	39:3A:159:GLN:HG2	1.88	0.55
2:S2:205:G:H2'	2:S2:206:G:H8	1.72	0.55
39:3A:175:HIS:CD2	39:3A:228:MET:HE2	2.42	0.55
39:3A:407:VAL:HA	39:3A:410:VAL:HG12	1.89	0.55
41:3C:460:GLN:NE2	41:3C:670:GLN:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:3E:309:GLN:HB2	42:3E:359:LYS:HE3	1.89	0.55
44:3G:269:TYR:HB2	44:3G:284:PHE:HB2	1.88	0.55
47:3K:44:LEU:HD21	48:3L:294:LEU:HD12	1.88	0.55
48:3L:256:VAL:HG23	48:3L:260:TYR:HD2	1.71	0.55
50:3N:413:LEU:HB3	50:3N:420:VAL:HG21	1.88	0.55
2:S2:885:U:O4	2:S2:901:G:O6	2.24	0.55
2:S2:943:U:OP1	4:SB:214:LYS:NZ	2.40	0.55
2:S2:1354:G:N2	2:S2:1357:A:OP2	2.38	0.55
3:SA:3:GLY:N	3:SA:56:GLU:OE2	2.38	0.55
29:SO:26:ASN:HD22	29:SO:125:LYS:HD3	1.71	0.55
48:3L:370:LEU:HD13	48:3L:373:ILE:HD11	1.87	0.55
2:S2:922:A:OP2	30:SW:3:ARG:NH2	2.39	0.55
3:SA:108:PHE:HB3	3:SA:140:VAL:HG11	1.88	0.55
21:Sc:14:VAL:HG13	21:Sc:53:GLY:H	1.72	0.55
25:SG:6:SER:HA	25:SG:13:GLN:HG2	1.87	0.55
41:3C:602:ASP:HB3	41:3C:605:VAL:HG22	1.89	0.55
44:3G:247:SER:HB3	44:3G:250:THR:HG23	1.89	0.55
2:S2:528:A:H2'	2:S2:529:A:C8	2.42	0.55
4:SB:224:GLU:OE1	4:SB:227:LYS:N	2.36	0.55
27:SM:42:LEU:O	27:SM:72:HIS:NE2	2.40	0.55
40:3B:576:LYS:HA	40:3B:593:HIS:HA	1.88	0.55
11:SL:23:VAL:HG12	11:SL:25:LEU:H	1.73	0.54
12:SP:34:MET:HE2	12:SP:42:ARG:HG3	1.88	0.54
22:Sd:21:CYS:HB3	22:Sd:26:ASN:H	1.73	0.54
48:3L:295:GLU:HB2	48:3L:298:GLU:HB2	1.89	0.54
8:SH:36:LEU:O	8:SH:40:LEU:HB3	2.08	0.54
39:3A:87:GLU:OE1	39:3A:91:ARG:NH1	2.40	0.54
39:3A:520:ARG:HB3	45:3H:234:ALA:HB2	1.88	0.54
47:3K:153:ILE:HB	47:3K:157:LEU:HD11	1.90	0.54
2:S2:1753:C:H5'	2:S2:1780:G:H22	1.72	0.54
12:SP:18:ARG:NH1	15:SS:88:LYS:O	2.40	0.54
15:SS:26:ILE:HA	15:SS:56:ALA:HB2	1.90	0.54
41:3C:641:ARG:NH2	50:3N:44:ASP:OD2	2.41	0.54
45:3H:123:THR:HG21	45:3H:128:PHE:HB3	1.90	0.54
2:S2:1838:U:O2	29:SO:150:ARG:NH1	2.40	0.54
9:SI:67:TRP:HD1	9:SI:189:VAL:HG11	1.73	0.54
13:SQ:9:SER:HA	13:SQ:25:CYS:O	2.08	0.54
13:SQ:11:GLN:HA	13:SQ:23:ALA:O	2.07	0.54
25:SG:88:ARG:HB2	25:SG:91:GLU:HB2	1.90	0.54
41:3C:662:GLN:HA	41:3C:665:VAL:HG12	1.90	0.54
42:3E:51:VAL:HG11	42:3E:74:ARG:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S2:1084:A:OP1	2:S2:1858:G:O2'	2.24	0.54
2:S2:1311:C:OP1	35:Sf:143:LYS:NZ	2.33	0.54
23:Sg:247:TRP:HA	23:Sg:259:TRP:O	2.07	0.54
26:SJ:3:VAL:HG13	26:SJ:5:ARG:HH11	1.73	0.54
39:3A:310:LEU:HG	39:3A:311:THR:HG22	1.88	0.54
39:3A:420:LYS:HD2	39:3A:421:GLU:HG2	1.89	0.54
2:S2:453:C:O2'	25:SG:92:ARG:O	2.24	0.54
2:S2:1130:G:OP2	2:S2:1130:G:N2	2.29	0.54
3:SA:52:LYS:HB2	14:SR:109:LEU:HD13	1.90	0.54
7:SF:30:ILE:HG23	7:SF:117:ILE:HD11	1.90	0.54
8:SH:80:VAL:HG23	8:SH:92:VAL:HG13	1.90	0.54
15:SS:124:ARG:O	15:SS:127:TRP:C	2.51	0.54
17:SU:21:ARG:HD3	17:SU:88:LEU:HD12	1.90	0.54
19:SX:77:ASN:O	19:SX:79:LYS:NZ	2.40	0.54
23:Sg:256:ILE:HB	23:Sg:270:LEU:HB2	1.89	0.54
42:3E:88:THR:HG21	42:3E:134:TYR:HB2	1.90	0.54
48:3L:388:LEU:O	48:3L:392:GLU:N	2.40	0.54
2:S2:752:G:OP1	2:S2:792:C:O2'	2.24	0.54
9:SI:25:ARG:HB2	9:SI:28:GLU:HG3	1.90	0.54
9:SI:151:GLU:HA	9:SI:154:LYS:HG2	1.89	0.54
2:S2:613:G:O2'	2:S2:627:U:OP2	2.25	0.53
2:S2:925:G:O6	2:S2:1017:U:O4	2.26	0.53
19:SX:84:PHE:HB3	19:SX:105:PHE:HE2	1.72	0.53
23:Sg:66:VAL:HA	23:Sg:82:SER:HA	1.89	0.53
42:3E:405:ILE:HA	42:3E:408:THR:HG22	1.90	0.53
49:3M:213:LYS:HD3	49:3M:268:LEU:HA	1.91	0.53
2:S2:67:C:OP1	25:SG:160:LYS:NZ	2.41	0.53
2:S2:571:U:O2'	31:SY:60:PHE:O	2.25	0.53
2:S2:1396:A:N7	2:S2:1449:G:O6	2.41	0.53
4:SB:190:PRO:HB3	39:3A:17:GLU:HG3	1.89	0.53
32:SZ:99:LEU:HG	32:SZ:109:TYR:HE1	1.72	0.53
37:4A:344:VAL:O	37:4A:372:ALA:HA	2.09	0.53
2:S2:289:G:OP1	6:SE:155:LYS:NZ	2.40	0.53
2:S2:1203:G:H1	2:S2:1696:C:H5	1.57	0.53
7:SF:90:VAL:HA	7:SF:93:VAL:HG12	1.91	0.53
39:3A:270:GLN:O	39:3A:274:ASN:ND2	2.41	0.53
48:3L:483:GLU:OE1	48:3L:489:GLN:NE2	2.41	0.53
2:S2:1584:G:OP1	16:ST:77:LYS:NZ	2.41	0.53
12:SP:91:GLY:N	12:SP:107:ILE:O	2.41	0.53
36:C1:97:LEU:O	36:C1:100:ILE:C	2.52	0.53
2:S2:1024:A:OP2	28:SN:124:ARG:NH2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:3C:744:MET:HE1	41:3C:787:SER:HA	1.91	0.53
42:3E:94:MET:HE3	42:3E:117:LEU:HD12	1.89	0.53
48:3L:232:HIS:O	48:3L:236:ASP:HB2	2.08	0.53
2:S2:835:C:N4	31:SY:9:THR:O	2.42	0.53
39:3A:483:ARG:NH2	41:3C:799:TYR:O	2.41	0.53
41:3C:68:ARG:NH1	41:3C:112:ASP:OD2	2.42	0.53
41:3C:336:ILE:O	41:3C:350:GLN:NE2	2.41	0.53
41:3C:815:LEU:HD12	41:3C:819:HIS:HE1	1.73	0.53
42:3E:262:ILE:O	42:3E:335:ASN:ND2	2.41	0.53
2:S2:795:A:H2'	2:S2:796:G:H8	1.74	0.53
4:SB:82:ARG:NH1	4:SB:191:ASP:OD2	2.42	0.53
41:3C:504:LEU:HB2	41:3C:564:ILE:HG23	1.91	0.53
41:3C:606:GLN:O	41:3C:610:ASN:ND2	2.42	0.53
41:3C:869:ASN:OD1	45:3H:261:ASN:ND2	2.41	0.53
2:S2:1562:C:H2'	2:S2:1563:G:C8	2.43	0.53
3:SA:37:TYR:OH	3:SA:57:LYS:NZ	2.42	0.53
15:SS:138:THR:HA	15:SS:141:ARG:HH21	1.74	0.53
41:3C:596:ASP:O	41:3C:599:GLN:NE2	2.42	0.53
42:3E:369:ARG:NH2	48:3L:480:ASP:OD1	2.42	0.53
47:3K:95:GLU:HG3	47:3K:100:ARG:HH21	1.73	0.53
2:S2:562:U:H2'	2:S2:563:G:C8	2.44	0.53
2:S2:969:U:O2	2:S2:971:G:N1	2.42	0.53
5:SD:195:THR:OG1	5:SD:197:LYS:NZ	2.41	0.53
9:SI:48:VAL:HG11	9:SI:54:LYS:HD2	1.91	0.53
23:Sg:188:HIS:HB3	23:Sg:219:TRP:HZ3	1.74	0.53
31:SY:29:HIS:O	31:SY:67:GLY:HA2	2.09	0.53
41:3C:326:HIS:HA	41:3C:329:VAL:HG12	1.89	0.53
43:3F:121:LEU:HB3	43:3F:167:GLU:HG2	1.91	0.53
47:3K:95:GLU:HA	47:3K:100:ARG:HE	1.74	0.53
2:S2:1548:G:O6	2:S2:1586:U:O4	2.26	0.53
5:SD:119:CYS:HA	5:SD:122:VAL:HG22	1.92	0.53
23:Sg:259:TRP:HD1	23:Sg:266:ILE:HA	1.74	0.53
2:S2:385:G:O2'	9:SI:10:LYS:NZ	2.41	0.52
2:S2:1650:A:H5''	13:SQ:139:ALA:HB2	1.92	0.52
26:SJ:94:LEU:HD23	26:SJ:97:ILE:HD12	1.90	0.52
2:S2:122:G:H21	6:SE:146:THR:HG21	1.74	0.52
23:Sg:166:VAL:HG12	23:Sg:176:VAL:HG22	1.90	0.52
37:4A:133:ALA:HA	37:4A:156:VAL:O	2.09	0.52
40:3B:486:ASP:HB2	40:3B:489:ILE:HB	1.91	0.52
45:3H:229:GLU:O	45:3H:232:SER:OG	2.28	0.52
2:S2:840:C:H4'	2:S2:841:G:H5''	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:SF:81:ARG:O	7:SF:85:LYS:NZ	2.34	0.52
2:S2:1004:U:H2'	2:S2:1005:G:H8	1.74	0.52
9:SI:149:TYR:HA	9:SI:152:ARG:HB2	1.91	0.52
29:SO:97:LEU:HD11	29:SO:112:ALA:HB1	1.91	0.52
45:3H:270:GLN:OE1	45:3H:274:LYS:NZ	2.42	0.52
47:3K:40:ASN:ND2	47:3K:132:THR:O	2.42	0.52
48:3L:256:VAL:O	48:3L:260:TYR:HB2	2.10	0.52
2:S2:880:G:O6	2:S2:906:U:O2	2.28	0.52
2:S2:1232:U:H2'	2:S2:1233:G:C8	2.45	0.52
2:S2:1424:G:H2'	2:S2:1425:G:H8	1.74	0.52
5:SD:213:PRO:HB3	14:SR:20:TYR:HE1	1.75	0.52
39:3A:336:THR:OG1	39:3A:340:ARG:NH1	2.42	0.52
39:3A:428:VAL:HA	39:3A:431:LEU:HD12	1.90	0.52
41:3C:733:MET:HA	41:3C:761:MET:HE1	1.92	0.52
42:3E:14:LEU:O	50:3N:10:GLN:NE2	2.42	0.52
15:SS:141:ARG:O	15:SS:144:ARG:O	2.27	0.52
23:Sg:199:THR:HG21	23:Sg:240:CYS:HA	1.91	0.52
26:SJ:67:ASP:HB3	26:SJ:70:ARG:HB3	1.92	0.52
31:SY:41:ARG:NH1	31:SY:52:PRO:O	2.42	0.52
49:3M:294:PHE:HB2	49:3M:330:ARG:HB3	1.92	0.52
12:SP:81:ARG:NH1	12:SP:120:SER:OG	2.42	0.52
23:Sg:214:GLY:HA2	23:Sg:236:ILE:HG12	1.91	0.52
2:S2:1398:G:H22	2:S2:1448:A:H2	1.58	0.52
13:SQ:19:ALA:HB2	13:SQ:75:GLY:HA3	1.92	0.52
45:3H:218:LEU:O	45:3H:222:SER:CB	2.58	0.52
2:S2:1353:A:OP1	3:SA:139:TYR:OH	2.26	0.52
41:3C:381:SER:HA	41:3C:384:ASP:HB2	1.90	0.52
2:S2:1436:C:O2'	2:S2:1438:A:OP2	2.26	0.52
3:SA:184:ARG:HB3	3:SA:191:ARG:HE	1.74	0.52
25:SG:181:THR:HG22	25:SG:184:VAL:HG23	1.92	0.52
26:SJ:103:GLU:O	26:SJ:107:GLU:HG2	2.10	0.52
42:3E:54:ALA:HB1	42:3E:70:LEU:HD21	1.91	0.52
49:3M:285:MET:HA	49:3M:288:GLU:HG2	1.92	0.52
2:S2:71:G:H2'	2:S2:72:C:H4'	1.91	0.51
2:S2:198:U:O2	2:S2:203:G:O6	2.28	0.51
26:SJ:146:SER:O	26:SJ:146:SER:OG	2.26	0.51
30:SW:32:LYS:O	30:SW:36:ARG:HG2	2.09	0.51
37:4A:274:GLN:HA	37:4A:324:ARG:O	2.09	0.51
41:3C:627:LYS:HA	41:3C:693:LEU:HD21	1.91	0.51
47:3K:20:ARG:HE	47:3K:49:ALA:HB2	1.75	0.51
2:S2:102:A:H4'	2:S2:104:A:C8	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S2:1580:A:OP1	17:SU:86:LYS:NZ	2.43	0.51
39:3A:373:ASP:OD1	39:3A:376:ARG:NH1	2.44	0.51
41:3C:773:ASP:OD1	41:3C:774:LYS:N	2.43	0.51
43:3F:95:HIS:HB2	43:3F:98:ILE:HG12	1.92	0.51
2:S2:492:C:OP2	31:SY:107:ARG:NH2	2.43	0.51
24:SC:184:VAL:HG11	24:SC:247:THR:HB	1.92	0.51
50:3N:222:ARG:HH11	50:3N:352:GLU:HA	1.74	0.51
50:3N:245:VAL:HG11	50:3N:495:ILE:HD11	1.93	0.51
2:S2:1548:G:C6	2:S2:1586:U:C4	2.98	0.51
16:ST:96:SER:HB3	16:ST:99:VAL:HG22	1.92	0.51
24:SC:272:HIS:O	24:SC:276:THR:OG1	2.21	0.51
39:3A:41:ARG:HH21	39:3A:77:ILE:HD11	1.74	0.51
43:3F:99:LEU:HD22	45:3H:218:LEU:HD21	1.92	0.51
48:3L:486:PHE:HA	48:3L:489:GLN:HB2	1.91	0.51
2:S2:868:G:OP2	2:S2:868:G:N2	2.35	0.51
2:S2:1486:A:H2'	2:S2:1487:A:C8	2.45	0.51
2:S2:1808:U:H2'	2:S2:1809:A:H8	1.76	0.51
17:SU:26:SER:OG	17:SU:27:ARG:N	2.44	0.51
21:Sc:21:THR:OG1	21:Sc:22:GLY:N	2.43	0.51
23:Sg:313:THR:HB	23:Sg:314:ILE:HD12	1.91	0.51
24:SC:130:ILE:HD13	24:SC:159:LYS:HG2	1.93	0.51
29:SO:98:ARG:HH21	29:SO:134:PRO:HG2	1.75	0.51
41:3C:340:ARG:NE	41:3C:384:ASP:OD2	2.42	0.51
42:3E:193:LYS:HE3	42:3E:214:LEU:HD21	1.91	0.51
48:3L:398:MET:HA	48:3L:401:MET:HE3	1.92	0.51
50:3N:526:THR:HG23	50:3N:527:PHE:HD1	1.76	0.51
2:S2:1127:C:O3'	33:Sb:17:ARG:NH1	2.44	0.51
42:3E:52:ASP:OD1	42:3E:52:ASP:N	2.43	0.51
42:3E:372:VAL:HG11	48:3L:481:LEU:HD11	1.93	0.51
49:3M:213:LYS:HZ3	49:3M:269:LEU:H	1.58	0.51
50:3N:270:GLN:NE2	50:3N:279:ASP:OD2	2.38	0.51
1:Ln:1:MET:HE1	1:Ln:9:ARG:HD3	1.93	0.51
2:S2:1535:U:O4	7:SF:159:ARG:NE	2.33	0.51
7:SF:49:LEU:HD21	13:SQ:47:LEU:HA	1.93	0.51
8:SH:138:GLU:H	8:SH:159:ASP:HB2	1.76	0.51
16:ST:42:HIS:HB3	16:ST:93:SER:HB2	1.93	0.51
43:3F:251:LEU:HD22	45:3H:162:LEU:HB2	1.93	0.51
11:SL:18:GLN:HA	11:SL:18:GLN:NE2	2.22	0.51
25:SG:85:ARG:HH12	31:SY:118:ARG:NE	2.09	0.51
39:3A:9:GLU:HG3	39:3A:46:ILE:HG12	1.91	0.51
39:3A:398:PHE:HD2	39:3A:509:PRO:HB2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:3E:183:ASP:HA	42:3E:186:MET:HE2	1.92	0.51
47:3K:216:SER:OG	48:3L:534:LYS:NZ	2.38	0.51
2:S2:307:G:N2	9:SI:45:THR:O	2.43	0.51
6:SE:11:ARG:HA	6:SE:28:ALA:HB2	1.93	0.51
6:SE:112:HIS:NE2	6:SE:237:SER:OG	2.38	0.51
39:3A:37:SER:O	39:3A:41:ARG:NH1	2.43	0.51
42:3E:39:GLN:HA	42:3E:42:LEU:HD12	1.92	0.51
50:3N:178:GLN:HA	50:3N:181:LYS:HG2	1.93	0.51
50:3N:269:VAL:O	50:3N:506:TYR:N	2.38	0.51
2:S2:837:A:N6	31:SY:9:THR:OG1	2.41	0.51
2:S2:921:G:OP1	33:Sb:26:GLN:NE2	2.43	0.51
2:S2:1036:A:N3	2:S2:1844:U:O2'	2.42	0.51
2:S2:1864:U:OP2	20:Sa:5:ARG:NH2	2.39	0.51
5:SD:45:ARG:HE	5:SD:83:SER:HA	1.77	0.51
11:SL:119:ASP:O	11:SL:147:LYS:NZ	2.44	0.51
15:SS:68:ILE:HG23	15:SS:72:GLN:HE22	1.76	0.51
38:CD:100:LEU:HD12	38:CD:100:LEU:C	2.34	0.51
49:3M:269:LEU:HD12	49:3M:272:GLN:H	1.75	0.51
2:S2:691:G:N2	2:S2:691:G:OP2	2.37	0.50
2:S2:1536:G:H2'	2:S2:1537:A:C8	2.44	0.50
3:SA:158:ASP:OD1	18:SV:65:SER:OG	2.24	0.50
23:Sg:212:LYS:HA	23:Sg:235:ILE:HG23	1.93	0.50
26:SJ:26:ASP:HB2	34:Se:42:PHE:HZ	1.76	0.50
39:3A:278:LYS:O	39:3A:281:THR:OG1	2.27	0.50
41:3C:672:PRO:HD2	41:3C:675:LEU:HD12	1.91	0.50
41:3C:815:LEU:O	41:3C:819:HIS:ND1	2.30	0.50
42:3E:36:GLU:HG3	50:3N:4:PHE:HB3	1.92	0.50
42:3E:384:ILE:HG13	42:3E:391:VAL:HG13	1.93	0.50
47:3K:101:GLN:NE2	47:3K:122:ASP:OD1	2.44	0.50
2:S2:67:C:OP2	25:SG:172:LYS:NZ	2.44	0.50
2:S2:1758:G:O2'	2:S2:1774:C:N4	2.44	0.50
18:SV:53:TYR:OH	18:SV:76:ASP:OD2	2.28	0.50
23:Sg:62:HIS:ND1	23:Sg:82:SER:HB3	2.25	0.50
25:SG:2:LYS:HB2	25:SG:108:VAL:HG23	1.93	0.50
27:SM:61:TYR:HH	27:SM:108:CYS:HG	1.55	0.50
31:SY:91:LEU:O	31:SY:94:HIS:O	2.30	0.50
39:3A:311:THR:OG1	39:3A:313:ASP:OD1	2.30	0.50
14:SR:104:GLU:HA	14:SR:107:LYS:HG2	1.94	0.50
39:3A:468:GLU:HA	39:3A:471:ILE:HG12	1.94	0.50
42:3E:32:TYR:HB2	50:3N:2:ALA:HA	1.94	0.50
48:3L:332:ALA:HA	48:3L:335:VAL:HG12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:SC:253:PRO:HA	24:SC:256:TRP:CG	2.47	0.50
26:SJ:114:VAL:HG23	26:SJ:119:LEU:HD13	1.94	0.50
39:3A:448:GLN:HB2	49:3M:324:LYS:HB3	1.91	0.50
49:3M:189:LEU:HB3	49:3M:226:LEU:HG	1.92	0.50
50:3N:301:ASP:OD2	50:3N:305:SER:OG	2.21	0.50
2:S2:907:G:H2'	2:S2:908:A:H8	1.75	0.50
2:S2:1280:G:H2'	2:S2:1281:G:H8	1.77	0.50
15:SS:4:VAL:HG13	15:SS:5:ILE:HG22	1.92	0.50
39:3A:264:LYS:HB3	39:3A:265:LYS:HZ2	1.77	0.50
40:3B:507:ARG:HB2	40:3B:547:PHE:HZ	1.76	0.50
45:3H:242:ASN:HD22	45:3H:330:ILE:HG22	1.76	0.50
2:S2:944:A:H5''	29:SO:134:PRO:HB3	1.92	0.50
4:SB:124:HIS:HA	4:SB:137:LEU:O	2.10	0.50
11:SL:17:PHE:O	11:SL:20:LYS:NZ	2.44	0.50
39:3A:464:ALA:HA	39:3A:467:LEU:HD12	1.93	0.50
40:3B:306:TYR:HA	40:3B:704:TRP:HA	1.94	0.50
42:3E:78:VAL:HA	42:3E:81:LEU:HD12	1.94	0.50
45:3H:134:LEU:HD11	45:3H:318:LEU:HD11	1.94	0.50
2:S2:561:A:O2'	26:SJ:134:HIS:NE2	2.36	0.50
3:SA:81:ASN:HA	3:SA:84:GLN:HB2	1.92	0.50
3:SA:200:ASP:HB2	14:SR:85:VAL:HG23	1.94	0.50
5:SD:226:GLN:HE22	23:Sg:225:LYS:HE2	1.76	0.50
25:SG:121:ILE:HG21	25:SG:124:LEU:HD22	1.93	0.50
41:3C:424:ILE:HG23	41:3C:425:LEU:H	1.76	0.50
42:3E:365:GLU:OE2	48:3L:474:LYS:NZ	2.44	0.50
49:3M:303:ILE:HB	49:3M:307:ASP:HB3	1.94	0.50
2:S2:1714:U:H2'	2:S2:1715:A:H8	1.76	0.50
16:ST:11:GLN:HA	16:ST:14:PHE:HB3	1.93	0.50
16:ST:76:THR:HG23	16:ST:94:ARG:HE	1.76	0.50
41:3C:712:LYS:HE2	41:3C:715:HIS:HD2	1.77	0.50
43:3F:272:VAL:HG11	45:3H:336:GLN:HE22	1.77	0.50
48:3L:490:LEU:O	48:3L:494:LYS:HG2	2.12	0.50
2:S2:201:C:H3'	2:S2:202:G:H21	1.78	0.49
6:SE:137:PRO:HB2	6:SE:150:PRO:HD2	1.93	0.49
13:SQ:85:ARG:NH2	13:SQ:118:THR:OG1	2.45	0.49
25:SG:57:ASP:OD1	25:SG:61:PHE:N	2.44	0.49
32:SZ:74:SER:HA	32:SZ:79:ILE:HB	1.94	0.49
2:S2:433:A:H5''	9:SI:22:HIS:HB3	1.94	0.49
2:S2:928:G:H2'	2:S2:929:G:C8	2.47	0.49
6:SE:208:VAL:HG21	6:SE:225:ILE:HD11	1.93	0.49
8:SH:76:GLN:HE21	8:SH:94:PHE:HB2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:SI:92:ARG:O	9:SI:94:LYS:NZ	2.46	0.49
30:SW:57:ARG:NH2	33:Sb:26:GLN:OE1	2.37	0.49
42:3E:136:LYS:HA	50:3N:16:TRP:HZ2	1.76	0.49
44:3G:243:VAL:HG22	44:3G:312:VAL:HG13	1.94	0.49
2:S2:207:G:H3'	2:S2:208:G:H8	1.78	0.49
2:S2:375:U:H2'	2:S2:376:A:C8	2.47	0.49
2:S2:533:A:H2'	2:S2:534:G:C8	2.47	0.49
13:SQ:39:LEU:HG	13:SQ:51:LEU:HD12	1.94	0.49
23:Sg:87:LEU:HB2	23:Sg:101:PHE:HB2	1.93	0.49
39:3A:350:GLU:OE1	39:3A:353:ARG:NE	2.44	0.49
45:3H:207:ASN:ND2	45:3H:212:ASN:OD1	2.45	0.49
50:3N:260:ARG:HB2	50:3N:430:TYR:HD2	1.77	0.49
2:S2:1286:G:N2	2:S2:1312:G:O2'	2.42	0.49
12:SP:24:GLN:O	12:SP:28:MET:HG3	2.13	0.49
49:3M:64:MET:HG3	49:3M:105:LEU:HD11	1.94	0.49
50:3N:329:ARG:HB2	50:3N:332:LYS:HD3	1.94	0.49
14:SR:1:MET:SD	14:SR:1:MET:N	2.79	0.49
17:SU:26:SER:HB3	17:SU:32:LEU:HD13	1.93	0.49
23:Sg:40:ILE:HB	23:Sg:59:LEU:HB2	1.94	0.49
41:3C:610:ASN:HD21	50:3N:43:ALA:HB3	1.78	0.49
41:3C:637:GLN:NE2	41:3C:682:LEU:HD23	2.27	0.49
32:SZ:74:SER:OG	32:SZ:79:ILE:O	2.24	0.49
39:3A:162:ASP:O	39:3A:165:ARG:NE	2.42	0.49
41:3C:576:HIS:O	41:3C:579:HIS:C	2.56	0.49
44:3G:243:VAL:HG13	44:3G:312:VAL:HG22	1.94	0.49
47:3K:7:MET:HB2	47:3K:32:TYR:HE1	1.77	0.49
12:SP:108:LYS:H	12:SP:111:MET:HE3	1.77	0.49
27:SM:18:LEU:HA	27:SM:21:VAL:HG22	1.95	0.49
34:Se:12:VAL:O	34:Se:16:THR:OG1	2.28	0.49
49:3M:292:ILE:HG23	49:3M:297:MET:HE3	1.93	0.49
50:3N:209:ILE:HD11	50:3N:214:GLU:HA	1.94	0.49
23:Sg:193:GLY:N	23:Sg:213:ASP:OD2	2.46	0.49
33:Sb:34:ASP:HB2	33:Sb:80:ARG:HB3	1.95	0.49
50:3N:396:LEU:HD12	50:3N:424:GLU:HG3	1.95	0.49
2:S2:1277:C:H2'	2:S2:1278:A:C8	2.48	0.49
12:SP:56:LEU:HD23	12:SP:60:LEU:HD23	1.95	0.49
13:SQ:117:ARG:HE	13:SQ:121:VAL:HG11	1.77	0.49
24:SC:155:ILE:O	24:SC:159:LYS:HG3	2.12	0.49
24:SC:187:ARG:HH12	24:SC:190:SER:HA	1.77	0.49
2:S2:1217:A:H2'	2:S2:1218:C:C6	2.48	0.49
2:S2:1588:A:H2'	2:S2:1589:A:C8	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:SF:88:MET:HG3	7:SF:91:ARG:HH21	1.78	0.49
12:SP:37:TYR:O	12:SP:42:ARG:NH1	2.45	0.49
15:SS:36:VAL:HG13	15:SS:40:TYR:HD2	1.78	0.49
19:SX:110:HIS:ND1	19:SX:111:ALA:O	2.46	0.49
44:3G:248:GLU:OE2	44:3G:279:SER:N	2.44	0.49
48:3L:360:ILE:O	48:3L:364:ASN:ND2	2.46	0.49
48:3L:386:ILE:HG13	48:3L:390:LEU:HD21	1.94	0.49
2:S2:907:G:H2'	2:S2:908:A:C8	2.48	0.48
2:S2:981:A:H2'	2:S2:982:G:C8	2.47	0.48
2:S2:1004:U:H2'	2:S2:1005:G:C8	2.48	0.48
6:SE:118:GLU:OE2	6:SE:237:SER:N	2.39	0.48
23:Sg:104:HIS:CE1	23:Sg:130:LYS:HG3	2.48	0.48
26:SJ:128:VAL:O	26:SJ:132:GLN:HG2	2.12	0.48
41:3C:667:ARG:HA	41:3C:670:GLN:HG2	1.94	0.48
43:3F:226:ARG:NH1	49:3M:13:ASP:OD2	2.46	0.48
48:3L:243:GLN:HG2	48:3L:253:PRO:HD2	1.95	0.48
50:3N:245:VAL:HG23	50:3N:371:LEU:HA	1.95	0.48
2:S2:302:A:N3	9:SI:64:ASN:ND2	2.60	0.48
3:SA:89:LYS:HB2	3:SA:202:TYR:CE1	2.48	0.48
4:SB:143:THR:OG1	4:SB:144:LYS:N	2.46	0.48
15:SS:81:ASP:OD1	15:SS:81:ASP:N	2.45	0.48
47:3K:11:VAL:HG13	47:3K:15:LEU:HD12	1.95	0.48
47:3K:162:LEU:HG	47:3K:170:LEU:HD11	1.95	0.48
48:3L:477:GLY:O	48:3L:481:LEU:HB2	2.13	0.48
2:S2:641:A:O2'	2:S2:645:C:OP1	2.30	0.48
2:S2:1850:A:H2'	2:S2:1851:A:C8	2.48	0.48
6:SE:115:THR:HG23	6:SE:118:GLU:H	1.78	0.48
12:SP:91:GLY:HA2	12:SP:107:ILE:O	2.13	0.48
39:3A:399:ASN:HA	49:3M:317:ARG:HH21	1.78	0.48
49:3M:251:SER:HA	49:3M:254:LYS:HG2	1.95	0.48
50:3N:432:LEU:HA	50:3N:435:TRP:HE3	1.78	0.48
2:S2:448:A:H5''	9:SI:25:ARG:HA	1.94	0.48
2:S2:1617:G:N1	2:S2:1620:A:OP2	2.46	0.48
2:S2:1861:G:H5''	20:Sa:3:LYS:HA	1.96	0.48
5:SD:131:ALA:HA	5:SD:191:PRO:HD3	1.94	0.48
10:SK:1:MET:HB3	10:SK:3:MET:HE3	1.96	0.48
12:SP:91:GLY:CA	12:SP:107:ILE:O	2.61	0.48
28:SN:140:LYS:HZ1	28:SN:142:GLU:HG2	1.79	0.48
39:3A:290:LEU:HA	39:3A:329:ILE:HG12	1.95	0.48
2:S2:197:U:OP2	2:S2:203:G:N2	2.46	0.48
2:S2:940:U:H3	2:S2:1002:U:H3	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:SI:152:ARG:O	9:SI:156:ALA:CB	2.61	0.48
27:SM:50:CYS:O	27:SM:76:LEU:HA	2.13	0.48
31:SY:79:LEU:HD11	31:SY:96:LEU:HD21	1.96	0.48
40:3B:310:PHE:HA	40:3B:699:PHE:HA	1.95	0.48
48:3L:245:GLU:HB3	48:3L:436:HIS:HD2	1.79	0.48
2:S2:218:U:O2	9:SI:184:ARG:NH1	2.43	0.48
2:S2:303:C:O2	9:SI:184:ARG:NH2	2.44	0.48
2:S2:463:C:O2	2:S2:466:G:N2	2.43	0.48
43:3F:142:SER:HB2	43:3F:145:GLU:HB3	1.95	0.48
47:3K:108:LEU:HB2	47:3K:113:HIS:HB2	1.96	0.48
47:3K:125:MET:HE3	47:3K:127:LEU:HB2	1.96	0.48
2:S2:198:U:O2	2:S2:203:G:C6	2.66	0.48
2:S2:1311:C:OP2	27:SM:36:ARG:NH2	2.46	0.48
6:SE:105:THR:O	6:SE:245:ARG:NH2	2.38	0.48
13:SQ:13:PHE:HA	13:SQ:22:VAL:HA	1.96	0.48
21:Sc:40:ARG:HH21	21:Sc:61:SER:HB3	1.79	0.48
22:Sd:26:ASN:HD22	22:Sd:27:ARG:H	1.60	0.48
41:3C:325:THR:OG1	41:3C:326:HIS:N	2.38	0.48
46:3I:111:SER:HA	46:3I:122:VAL:HA	1.96	0.48
50:3N:383:GLY:HA3	50:3N:387:GLU:HG3	1.95	0.48
2:S2:4:C:H4'	24:SC:207:ALA:HB2	1.95	0.48
8:SH:69:LEU:HD13	8:SH:96:ALA:HB2	1.96	0.48
16:ST:2:PRO:HA	16:ST:3:GLY:HA3	1.74	0.48
22:Sd:42:CYS:HA	22:Sd:45:GLN:HB2	1.95	0.48
27:SM:92:CYS:HB3	27:SM:94:ILE:HG12	1.96	0.48
45:3H:325:THR:O	45:3H:329:ASN:ND2	2.46	0.48
49:3M:64:MET:HE2	49:3M:101:LEU:HD21	1.96	0.48
1:Ln:10:MET:SD	2:S2:1172:U:H5''	2.54	0.48
2:S2:1714:U:H2'	2:S2:1715:A:C8	2.49	0.48
8:SH:126:HIS:HA	8:SH:129:ILE:HG22	1.95	0.48
25:SG:159:ARG:HE	25:SG:173:ALA:HB2	1.78	0.48
30:SW:14:ILE:HG22	30:SW:25:VAL:HG11	1.95	0.48
41:3C:370:VAL:HB	41:3C:431:LEU:HD12	1.95	0.48
42:3E:111:ARG:O	42:3E:111:ARG:NH1	2.46	0.48
42:3E:306:ASP:OD1	42:3E:307:GLY:N	2.47	0.48
2:S2:668:A:H5''	2:S2:1198:G:H4'	1.96	0.48
9:SI:110:ARG:HG3	9:SI:121:LEU:HD23	1.94	0.48
17:SU:97:ILE:HD12	17:SU:100:GLN:HE21	1.79	0.48
24:SC:128:VAL:HG11	24:SC:155:ILE:HG22	1.95	0.48
39:3A:335:ARG:HH21	41:3C:745:LYS:HB3	1.79	0.48
42:3E:422:ILE:HA	42:3E:425:LYS:HG2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:3F:334:LEU:HA	43:3F:337:VAL:HG12	1.94	0.48
45:3H:62:VAL:HG22	45:3H:123:THR:HA	1.96	0.48
45:3H:124:TYR:HE2	45:3H:245:LEU:HD11	1.79	0.48
45:3H:151:ILE:HD13	45:3H:167:TYR:HD2	1.79	0.48
47:3K:84:LEU:O	47:3K:88:MET:HG2	2.13	0.48
2:S2:329:G:H2'	2:S2:330:G:C8	2.48	0.47
2:S2:563:G:H1	2:S2:592:C:H5	1.62	0.47
2:S2:1741:U:N3	2:S2:1794:C:N4	2.61	0.47
11:SL:18:GLN:HE21	11:SL:18:GLN:CA	2.20	0.47
20:Sa:47:ALA:HA	20:Sa:50:VAL:HB	1.95	0.47
25:SG:65:GLN:HE21	25:SG:65:GLN:HB2	1.55	0.47
26:SJ:149:VAL:HG11	26:SJ:157:ILE:HD11	1.95	0.47
39:3A:380:LEU:O	39:3A:388:LYS:NZ	2.37	0.47
43:3F:169:ILE:HG13	43:3F:195:PRO:HG3	1.96	0.47
2:S2:1543:U:OP2	16:ST:62:ARG:NH2	2.36	0.47
6:SE:175:PHE:HE2	6:SE:198:ARG:HD2	1.78	0.47
27:SM:89:VAL:HG21	27:SM:109:VAL:HG21	1.95	0.47
42:3E:151:LEU:HD11	50:3N:16:TRP:HZ3	1.78	0.47
48:3L:336:PHE:HA	48:3L:339:ILE:HG22	1.97	0.47
3:SA:33:GLN:NE2	18:SV:64:GLU:OE2	2.48	0.47
7:SF:165:ASN:OD1	7:SF:166:ILE:N	2.47	0.47
39:3A:489:ARG:HH12	41:3C:806:THR:HG21	1.79	0.47
41:3C:637:GLN:HE21	41:3C:682:LEU:HD23	1.80	0.47
42:3E:186:MET:HA	42:3E:189:LEU:HD12	1.96	0.47
49:3M:46:ILE:HG21	49:3M:82:LEU:HD11	1.96	0.47
49:3M:120:ARG:HH22	49:3M:150:TRP:HE1	1.62	0.47
49:3M:290:LYS:HE3	49:3M:336:HIS:HA	1.96	0.47
2:S2:996:A:H2'	2:S2:997:A:C8	2.49	0.47
13:SQ:16:LYS:HG2	13:SQ:79:ALA:HA	1.96	0.47
39:3A:324:LEU:HD12	39:3A:424:LEU:HD13	1.95	0.47
41:3C:499:VAL:HA	41:3C:502:ILE:HG22	1.96	0.47
47:3K:102:ILE:HD11	47:3K:125:MET:HE1	1.97	0.47
50:3N:21:VAL:HG12	50:3N:26:ARG:NH1	2.29	0.47
2:S2:223:C:H2'	2:S2:224:A:C8	2.49	0.47
2:S2:656:G:N2	2:S2:663:C:H5''	2.29	0.47
27:SM:69:CYS:O	27:SM:72:HIS:C	2.57	0.47
38:CD:100:LEU:HD12	38:CD:101:ASP:CA	2.43	0.47
39:3A:559:LYS:O	39:3A:563:LYS:NZ	2.47	0.47
42:3E:399:SER:O	42:3E:403:GLN:NE2	2.48	0.47
47:3K:192:GLN:NE2	48:3L:512:GLU:OE2	2.48	0.47
48:3L:384:GLU:HB3	48:3L:525:LYS:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S2:503:C:H3'	2:S2:504:G:H8	1.80	0.47
2:S2:557:U:H2'	2:S2:558:G:C8	2.49	0.47
2:S2:1013:U:OP1	2:S2:1129:G:O2'	2.29	0.47
2:S2:1261:C:O2	22:Sd:10:HIS:NE2	2.39	0.47
6:SE:45:ILE:HB	6:SE:80:ILE:HG23	1.97	0.47
25:SG:134:GLY:HA3	25:SG:158:VAL:HG11	1.97	0.47
27:SM:23:LYS:HA	27:SM:23:LYS:HD3	1.70	0.47
39:3A:228:MET:HA	39:3A:231:GLU:HG3	1.97	0.47
42:3E:215:ILE:HD11	42:3E:242:TYR:HB3	1.97	0.47
50:3N:200:GLU:HB2	50:3N:328:LEU:HD23	1.96	0.47
2:S2:1025:U:OP1	2:S2:1090:C:O2'	2.32	0.47
2:S2:1230:C:OP1	15:SS:130:ARG:NH2	2.47	0.47
2:S2:1556:A:N6	22:Sd:13:LYS:HA	2.30	0.47
3:SA:82:THR:O	3:SA:82:THR:OG1	2.30	0.47
8:SH:145:ARG:NH2	30:SW:49:GLU:OE1	2.46	0.47
9:SI:67:TRP:HE3	9:SI:72:CYS:HB3	1.80	0.47
14:SR:20:TYR:HE2	14:SR:38:ILE:HB	1.80	0.47
14:SR:32:LYS:HD2	14:SR:47:ARG:HH21	1.80	0.47
19:SX:67:ARG:NH2	19:SX:114:ASP:OD2	2.34	0.47
25:SG:137:ARG:HD2	25:SG:178:ARG:HD2	1.96	0.47
27:SM:15:ASN:OD1	27:SM:16:THR:N	2.47	0.47
29:SO:101:GLY:HA2	29:SO:106:LYS:HD3	1.96	0.47
41:3C:582:TRP:HE1	41:3C:616:LEU:HG	1.79	0.47
41:3C:648:GLN:HE22	41:3C:677:ILE:H	1.63	0.47
42:3E:211:ARG:O	42:3E:215:ILE:HG12	2.14	0.47
42:3E:270:ARG:HA	42:3E:273:VAL:HG12	1.97	0.47
43:3F:309:MET:HA	43:3F:312:VAL:HG22	1.97	0.47
48:3L:367:MET:HA	48:3L:370:LEU:HB2	1.97	0.47
48:3L:544:ILE:HA	48:3L:547:ILE:HG12	1.97	0.47
2:S2:375:U:H2'	2:S2:376:A:H8	1.80	0.47
5:SD:70:THR:HG22	5:SD:86:LEU:HD13	1.97	0.47
5:SD:213:PRO:HB3	14:SR:20:TYR:CE1	2.50	0.47
12:SP:44:ARG:O	12:SP:47:ARG:C	2.58	0.47
24:SC:70:VAL:HG11	24:SC:93:ILE:HG12	1.97	0.47
26:SJ:38:ARG:NH1	26:SJ:42:GLU:OE2	2.48	0.47
30:SW:11:LEU:HD12	30:SW:74:VAL:HB	1.96	0.47
41:3C:375:LYS:HB3	41:3C:408:LEU:HD12	1.97	0.47
44:3G:289:ARG:HG3	44:3G:291:GLU:H	1.80	0.47
48:3L:279:ARG:HA	48:3L:282:SER:HB2	1.97	0.47
2:S2:145:G:H2'	2:S2:146:G:C8	2.50	0.47
2:S2:186:C:H2'	2:S2:187:G:H8	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S2:932:G:O2'	2:S2:934:G:OP2	2.32	0.47
2:S2:1221:G:O2'	2:S2:1676:U:O2	2.28	0.47
25:SG:216:ARG:O	25:SG:217:MET:HG3	2.15	0.47
39:3A:153:LEU:HD23	39:3A:184:PHE:CE1	2.50	0.47
43:3F:265:LEU:HB2	45:3H:203:ILE:HB	1.95	0.47
45:3H:218:LEU:O	45:3H:222:SER:OG	2.29	0.47
2:S2:165:G:OP2	2:S2:165:G:N2	2.40	0.47
2:S2:1329:U:O4	2:S2:1493:C:O2'	2.30	0.47
3:SA:123:VAL:HG22	3:SA:145:ILE:HB	1.97	0.47
7:SF:201:LYS:HA	7:SF:204:ARG:NE	2.30	0.47
25:SG:33:ALA:HA	25:SG:51:ARG:HG3	1.97	0.47
29:SO:12:GLU:HA	29:SO:13:GLN:HA	1.65	0.47
41:3C:695:ILE:HG21	41:3C:744:MET:HG3	1.97	0.47
49:3M:292:ILE:HB	49:3M:332:VAL:HB	1.97	0.47
5:SD:67:ARG:HD3	10:SK:96:ARG:HB2	1.96	0.46
24:SC:271:ASP:OD1	24:SC:271:ASP:N	2.43	0.46
27:SM:80:ASP:OD1	27:SM:81:ASP:N	2.46	0.46
27:SM:120:ALA:O	27:SM:124:ILE:HG12	2.15	0.46
32:SZ:99:LEU:HD23	32:SZ:102:LYS:HB2	1.96	0.46
41:3C:570:LEU:HD21	41:3C:594:LEU:HG	1.96	0.46
2:S2:449:A:N1	25:SG:88:ARG:NH2	2.64	0.46
2:S2:1806:A:H2'	2:S2:1807:C:C6	2.51	0.46
24:SC:183:LYS:HG2	30:SW:95:PRO:HA	1.97	0.46
41:3C:324:ILE:HG22	41:3C:325:THR:H	1.80	0.46
42:3E:413:PHE:O	42:3E:416:GLN:HG3	2.15	0.46
49:3M:47:GLU:OE2	49:3M:89:LYS:NZ	2.44	0.46
49:3M:120:ARG:HA	49:3M:123:VAL:HG12	1.97	0.46
2:S2:614:C:O2'	2:S2:626:G:N2	2.48	0.46
2:S2:1550:G:H3'	2:S2:1579:A:H61	1.80	0.46
3:SA:110:ASN:HB3	3:SA:113:GLN:HG3	1.98	0.46
8:SH:81:ARG:HG2	8:SH:85:LYS:NZ	2.31	0.46
24:SC:166:ARG:HB2	24:SC:248:TYR:CD1	2.49	0.46
26:SJ:81:LEU:HA	26:SJ:84:ILE:HG22	1.97	0.46
42:3E:189:LEU:O	42:3E:193:LYS:HG2	2.16	0.46
45:3H:123:THR:OG1	45:3H:127:SER:O	2.33	0.46
2:S2:17:C:O2'	2:S2:1194:A:N1	2.45	0.46
2:S2:980:A:H2'	2:S2:981:A:C8	2.51	0.46
2:S2:1819:A:H2'	2:S2:1820:G:C8	2.50	0.46
5:SD:136:VAL:HG22	5:SD:186:VAL:HG23	1.97	0.46
6:SE:15:PRO:HG3	6:SE:39:ARG:HD2	1.97	0.46
31:SY:26:ASP:HA	31:SY:69:THR:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:SY:62:THR:HA	31:SY:69:THR:HA	1.98	0.46
41:3C:837:GLN:O	41:3C:840:GLN:NE2	2.48	0.46
2:S2:942:G:H2'	2:S2:943:U:C6	2.51	0.46
3:SA:159:ILE:HD11	18:SV:34:MET:HE1	1.98	0.46
15:SS:6:PRO:HG2	15:SS:58:GLU:HG2	1.97	0.46
20:Sa:49:ALA:HB1	29:SO:117:ARG:HD3	1.97	0.46
23:Sg:5:MET:HB3	23:Sg:270:LEU:HD21	1.96	0.46
39:3A:383:VAL:HB	39:3A:388:LYS:HD3	1.97	0.46
45:3H:231:LEU:HA	45:3H:340:LYS:HG2	1.97	0.46
47:3K:29:LEU:HD11	47:3K:46:ALA:HB1	1.98	0.46
49:3M:193:THR:OG1	49:3M:195:ASP:OD1	2.29	0.46
2:S2:1119:A:H5''	2:S2:1120:U:C5	2.50	0.46
4:SB:28:LYS:HA	4:SB:50:THR:HA	1.98	0.46
14:SR:97:GLU:N	14:SR:97:GLU:OE1	2.48	0.46
43:3F:115:ARG:C	43:3F:139:HIS:HE2	2.24	0.46
48:3L:330:GLN:O	48:3L:334:ARG:NH1	2.41	0.46
2:S2:328:U:O2'	2:S2:329:G:O5'	2.33	0.46
2:S2:1268:C:HO2'	12:SP:97:TYR:HH	1.61	0.46
2:S2:1579:A:O2'	2:S2:1581:C:OP2	2.26	0.46
7:SF:175:ASP:HA	7:SF:178:ILE:HG22	1.96	0.46
9:SI:135:GLU:O	9:SI:139:LYS:HG3	2.16	0.46
13:SQ:53:GLU:O	13:SQ:57:LEU:CB	2.63	0.46
23:Sg:69:VAL:HA	23:Sg:79:LEU:O	2.16	0.46
33:Sb:74:THR:HG22	33:Sb:75:GLU:H	1.80	0.46
39:3A:244:GLU:HB3	39:3A:246:TRP:CH2	2.50	0.46
42:3E:266:ASP:HB3	42:3E:269:LYS:HE2	1.97	0.46
45:3H:63:VAL:HG22	45:3H:122:SER:OG	2.15	0.46
48:3L:348:SER:HB3	48:3L:352:ARG:HB2	1.97	0.46
48:3L:373:ILE:HG22	48:3L:401:MET:HE1	1.97	0.46
2:S2:557:U:H5'	2:S2:558:G:H8	1.80	0.46
2:S2:1128:C:P	33:Sb:17:ARG:HH12	2.39	0.46
42:3E:111:ARG:HA	42:3E:111:ARG:HD2	1.84	0.46
45:3H:281:ARG:O	45:3H:285:ASN:ND2	2.49	0.46
2:S2:1189:A:H2'	2:S2:1190:A:C8	2.51	0.46
11:SL:28:THR:HA	11:SL:29:GLY:HA2	1.62	0.46
18:SV:77:GLY:HA2	18:SV:81:LYS:HE3	1.98	0.46
29:SO:100:THR:HG21	29:SO:104:ARG:HE	1.81	0.46
48:3L:432:HIS:CD2	48:3L:433:PRO:HD2	2.51	0.46
2:S2:441:C:H2'	2:S2:442:C:C6	2.50	0.46
2:S2:880:G:O6	2:S2:906:U:C2	2.69	0.46
2:S2:1752:C:N4	2:S2:1779:G:N2	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:SD:67:ARG:O	5:SD:70:THR:OG1	2.29	0.46
16:ST:28:LEU:HA	16:ST:110:LEU:HD21	1.98	0.46
16:ST:56:ARG:HA	16:ST:56:ARG:HD3	1.81	0.46
39:3A:19:LEU:HD21	39:3A:57:LEU:HD21	1.97	0.46
42:3E:163:ARG:HD3	42:3E:164:ASN:HB2	1.97	0.46
45:3H:123:THR:OG1	45:3H:124:TYR:N	2.49	0.46
45:3H:250:VAL:HA	45:3H:253:MET:HG3	1.97	0.46
2:S2:795:A:H2'	2:S2:796:G:C8	2.51	0.45
6:SE:92:ILE:O	6:SE:94:LYS:N	2.47	0.45
13:SQ:50:LYS:HA	13:SQ:50:LYS:HD3	1.82	0.45
26:SJ:121:LYS:HG2	40:3B:510:PHE:HD2	1.80	0.45
32:SZ:98:LYS:NZ	32:SZ:112:ASN:HA	2.31	0.45
42:3E:264:ASN:OD1	42:3E:270:ARG:NH1	2.49	0.45
43:3F:244:THR:HA	43:3F:247:ILE:HG22	1.97	0.45
46:3I:288:ILE:HA	46:3I:304:GLY:HA2	1.97	0.45
2:S2:168:C:H5'	25:SG:131:ARG:HH11	1.81	0.45
23:Sg:258:ILE:HB	23:Sg:268:ASP:HB2	1.98	0.45
30:SW:101:PHE:HA	30:SW:113:HIS:HE1	1.81	0.45
39:3A:267:PRO:HG2	39:3A:272:MET:SD	2.56	0.45
43:3F:217:VAL:O	43:3F:233:THR:OG1	2.34	0.45
45:3H:245:LEU:HB3	45:3H:249:ARG:HH21	1.81	0.45
45:3H:345:GLN:NE2	45:3H:349:GLU:OE1	2.50	0.45
48:3L:541:ASP:HA	48:3L:544:ILE:HG12	1.97	0.45
1:Ln:1:MET:HB3	1:Ln:6:ARG:HH12	1.81	0.45
8:SH:30:LEU:HD21	8:SH:79:LEU:HD22	1.97	0.45
23:Sg:173:LEU:HD21	23:Sg:175:LYS:HE3	1.99	0.45
27:SM:64:LEU:HD11	35:Sf:106:TYR:HD2	1.80	0.45
31:SY:114:MET:HA	31:SY:117:VAL:HG12	1.97	0.45
39:3A:286:SER:HA	41:3C:728:GLY:HA2	1.98	0.45
39:3A:597:ARG:NH1	39:3A:598:GLU:OE2	2.49	0.45
41:3C:659:ASN:HA	41:3C:662:GLN:HE22	1.81	0.45
42:3E:307:GLY:HA2	42:3E:310:LYS:HG2	1.97	0.45
43:3F:327:LEU:HD13	47:3K:204:LYS:HE2	1.98	0.45
43:3F:341:ALA:HB1	45:3H:327:CYS:SG	2.57	0.45
2:S2:198:U:H2'	2:S2:199:C:H2'	1.99	0.45
2:S2:1171:G:O2'	2:S2:1187:G:O6	2.25	0.45
2:S2:1435:C:H41	17:SU:92:HIS:CE1	2.35	0.45
2:S2:1497:G:O6	10:SK:25:LYS:NZ	2.45	0.45
2:S2:1556:A:O2'	2:S2:1557:C:O4'	2.31	0.45
2:S2:1562:C:H5''	16:ST:71:GLY:HA3	1.99	0.45
19:SX:49:GLY:O	19:SX:99:GLU:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:3C:418:ILE:HG12	41:3C:438:LEU:HD23	1.97	0.45
42:3E:371:ILE:HA	42:3E:374:LEU:HD12	1.98	0.45
43:3F:306:ARG:NH2	49:3M:219:LEU:HD11	2.31	0.45
45:3H:218:LEU:O	45:3H:222:SER:HB2	2.15	0.45
50:3N:249:ASP:OD2	50:3N:376:GLU:N	2.42	0.45
3:SA:91:ALA:O	3:SA:94:THR:C	2.60	0.45
3:SA:169:HIS:HA	3:SA:203:PHE:CD1	2.51	0.45
12:SP:57:LEU:O	12:SP:61:ARG:HG3	2.17	0.45
15:SS:1:MET:HG3	32:SZ:49:LEU:HD11	1.98	0.45
15:SS:35:GLY:O	15:SS:97:GLN:NE2	2.50	0.45
19:SX:88:ASP:HB3	34:Se:10:GLY:HA2	1.98	0.45
29:SO:36:SER:C	29:SO:38:ASN:H	2.25	0.45
40:3B:516:LYS:HE2	40:3B:529:LYS:HB3	1.99	0.45
42:3E:189:LEU:HD11	42:3E:221:VAL:HG11	1.98	0.45
42:3E:234:ASP:HA	42:3E:238:TYR:HD2	1.80	0.45
43:3F:242:TYR:H	43:3F:245:GLU:HB2	1.81	0.45
45:3H:113:ASP:OD1	45:3H:113:ASP:N	2.49	0.45
45:3H:262:THR:O	45:3H:266:ASN:ND2	2.50	0.45
50:3N:190:PRO:HA	50:3N:362:ARG:O	2.16	0.45
4:SB:119:THR:H	4:SB:143:THR:HG22	1.81	0.45
11:SL:7:GLU:HG2	11:SL:8:ARG:H	1.81	0.45
15:SS:3:LEU:HD12	15:SS:4:VAL:HG12	1.98	0.45
23:Sg:68:ASP:O	23:Sg:80:SER:HA	2.17	0.45
27:SM:86:GLY:HA3	27:SM:105:GLY:HA3	1.97	0.45
41:3C:557:ALA:HB2	50:3N:27:ASP:HB3	1.98	0.45
44:3G:289:ARG:HE	44:3G:290:ARG:H	1.64	0.45
45:3H:227:LYS:HD2	45:3H:230:LEU:HD23	1.98	0.45
49:3M:205:HIS:HE1	49:3M:236:LEU:HD21	1.81	0.45
50:3N:393:ILE:O	50:3N:394:LYS:HD2	2.17	0.45
2:S2:1216:C:HO2'	13:SQ:145:TYR:HH	1.65	0.45
2:S2:1421:A:H5''	2:S2:1422:G:C4	2.51	0.45
13:SQ:5:GLY:N	13:SQ:27:ARG:HH22	2.15	0.45
15:SS:59:LEU:HD12	15:SS:63:GLU:HG3	1.98	0.45
26:SJ:140:GLN:NE2	31:SY:64:PHE:O	2.50	0.45
41:3C:480:CYS:HA	41:3C:483:ILE:HG22	1.98	0.45
42:3E:299:LEU:HD13	42:3E:340:ILE:HG22	1.99	0.45
2:S2:186:C:H2'	2:S2:187:G:C8	2.52	0.45
23:Sg:34:ALA:HB2	23:Sg:69:VAL:HG13	1.99	0.45
24:SC:77:SER:O	24:SC:80:GLU:N	2.39	0.45
37:4A:245:GLY:O	37:4A:369:LYS:N	2.50	0.45
39:3A:250:PHE:HB2	41:3C:726:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:3A:367:ARG:O	39:3A:371:ILE:HG12	2.17	0.45
41:3C:96:ILE:HG13	41:3C:97:VAL:H	1.81	0.45
41:3C:515:ASP:OD1	41:3C:515:ASP:N	2.44	0.45
45:3H:269:LYS:HA	45:3H:269:LYS:HD3	1.79	0.45
2:S2:483:C:H5'	19:SX:48:LYS:HG3	1.98	0.45
2:S2:1736:G:H2'	2:S2:1737:G:C8	2.52	0.45
25:SG:85:ARG:HH12	31:SY:118:ARG:HE	1.65	0.45
38:CD:106:SER:C	38:CD:108:LYS:H	2.24	0.45
47:3K:7:MET:HB2	47:3K:32:TYR:CE1	2.52	0.45
50:3N:199:LEU:O	50:3N:335:TYR:N	2.49	0.45
50:3N:215:LYS:HB3	50:3N:215:LYS:HE2	1.72	0.45
2:S2:57:U:OP1	2:S2:504:G:O2'	2.33	0.45
2:S2:1521:C:OP2	15:SS:136:THR:OG1	2.35	0.45
6:SE:71:LYS:HA	6:SE:76:VAL:HA	1.99	0.45
11:SL:22:ARG:NH2	11:SL:28:THR:OG1	2.50	0.45
15:SS:119:ALA:O	15:SS:123:LEU:HB2	2.17	0.45
25:SG:84:TYR:HD1	25:SG:95:LYS:HD2	1.82	0.45
31:SY:91:LEU:O	31:SY:94:HIS:C	2.60	0.45
47:3K:90:ASP:O	47:3K:94:GLN:HB2	2.16	0.45
47:3K:139:ARG:NH2	47:3K:169:GLN:OE1	2.50	0.45
48:3L:312:GLN:HA	48:3L:315:THR:HG22	1.98	0.45
50:3N:497:ILE:HA	50:3N:500:LYS:HG2	1.99	0.45
2:S2:380:G:P	9:SI:56:ARG:HH22	2.40	0.44
2:S2:874:G:H2'	2:S2:875:A:H8	1.81	0.44
2:S2:1220:A:N3	2:S2:1677:U:O2'	2.40	0.44
13:SQ:13:PHE:HB3	13:SQ:22:VAL:HG12	1.99	0.44
23:Sg:10:THR:HG21	23:Sg:306:LEU:HD23	1.99	0.44
26:SJ:87:LEU:HD13	26:SJ:100:LEU:HD21	1.99	0.44
43:3F:132:THR:OG1	43:3F:167:GLU:OE2	2.35	0.44
2:S2:15:U:H2'	2:S2:16:G:O4'	2.17	0.44
2:S2:152:U:O4'	25:SG:132:ARG:NH1	2.51	0.44
26:SJ:106:LEU:HD23	26:SJ:109:ARG:HD2	1.99	0.44
26:SJ:179:LYS:HA	26:SJ:182:GLN:HG2	1.99	0.44
39:3A:327:LEU:O	39:3A:434:ASN:ND2	2.50	0.44
42:3E:334:GLU:O	42:3E:338:LEU:HG	2.17	0.44
43:3F:118:GLY:HA3	43:3F:173:TYR:CZ	2.51	0.44
2:S2:562:U:O4	26:SJ:172:ARG:NH2	2.50	0.44
2:S2:690:G:OP2	2:S2:690:G:N2	2.45	0.44
8:SH:87:PHE:HB3	8:SH:90:LYS:HE2	1.99	0.44
11:SL:77:VAL:HG22	11:SL:86:ILE:HD12	1.99	0.44
21:Sc:44:ARG:HD2	21:Sc:44:ARG:HA	1.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:3A:591:LYS:HA	39:3A:591:LYS:HD2	1.82	0.44
40:3B:327:VAL:HA	40:3B:328:SER:HA	1.58	0.44
49:3M:313:ILE:O	49:3M:317:ARG:HG2	2.16	0.44
50:3N:232:ASP:HB3	50:3N:235:ILE:HB	1.99	0.44
2:S2:902:G:O2'	2:S2:903:A:O4'	2.35	0.44
2:S2:1839:U:H2'	2:S2:1840:U:C6	2.52	0.44
13:SQ:113:ILE:HD12	13:SQ:117:ARG:HG3	2.00	0.44
18:SV:3:ASN:HA	24:SC:173:LYS:HD3	2.00	0.44
26:SJ:84:ILE:HD11	26:SJ:148:ILE:HG21	1.99	0.44
41:3C:490:LEU:HD12	41:3C:502:ILE:HG21	1.99	0.44
43:3F:328:ASN:HA	43:3F:331:ILE:HG12	1.99	0.44
49:3M:362:ASN:O	49:3M:366:ASN:ND2	2.50	0.44
50:3N:248:THR:H	50:3N:251:ILE:HD11	1.82	0.44
2:S2:551:U:H2'	2:S2:552:G:C4	2.52	0.44
2:S2:1600:G:H4'	32:SZ:43:LYS:HE3	1.99	0.44
6:SE:229:GLY:HA3	6:SE:234:PRO:HA	2.00	0.44
25:SG:98:ARG:NH2	25:SG:103:ASP:OD1	2.50	0.44
28:SN:140:LYS:NZ	28:SN:142:GLU:HG2	2.32	0.44
50:3N:200:GLU:OE2	50:3N:334:ARG:NH2	2.50	0.44
2:S2:118:C:H1'	2:S2:445:A:C5	2.53	0.44
2:S2:482:G:H5'	19:SX:76:LYS:HB3	1.98	0.44
2:S2:495:U:H2'	2:S2:496:C:O4'	2.18	0.44
2:S2:1438:A:H2'	2:S2:1439:A:C8	2.52	0.44
9:SI:81:VAL:HG12	9:SI:102:VAL:HG12	2.00	0.44
27:SM:55:ASN:HB2	27:SM:81:ASP:HA	2.00	0.44
31:SY:38:THR:O	31:SY:42:GLU:HG2	2.18	0.44
31:SY:80:ASP:OD1	31:SY:81:TYR:N	2.50	0.44
47:3K:8:ARG:HA	47:3K:8:ARG:HD3	1.80	0.44
48:3L:431:VAL:HA	48:3L:434:ASN:HA	1.99	0.44
2:S2:1566:G:O6	16:ST:101:ARG:NH2	2.51	0.44
18:SV:17:CYS:O	18:SV:21:ASN:N	2.51	0.44
39:3A:257:HIS:NE2	39:3A:357:THR:O	2.50	0.44
41:3C:504:LEU:HD22	41:3C:564:ILE:HG12	1.99	0.44
41:3C:758:ASN:N	41:3C:758:ASN:OD1	2.49	0.44
43:3F:231:MET:SD	43:3F:231:MET:N	2.91	0.44
50:3N:252:LEU:O	50:3N:256:MET:CB	2.59	0.44
2:S2:1628:C:H2'	2:S2:1629:C:C6	2.52	0.44
2:S2:1744:G:H1'	2:S2:1790:A:N6	2.33	0.44
2:S2:1786:U:O2'	2:S2:1787:G:H8	2.01	0.44
5:SD:195:THR:HG23	5:SD:197:LYS:HG2	2.00	0.44
14:SR:14:ARG:O	14:SR:18:GLU:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Sd:3:HIS:CE1	22:Sd:5:GLN:HB2	2.53	0.44
41:3C:745:LYS:HA	41:3C:745:LYS:HD2	1.81	0.44
50:3N:328:LEU:HD11	50:3N:393:ILE:HG13	2.00	0.44
2:S2:1232:U:H2'	2:S2:1233:G:H8	1.83	0.44
3:SA:51:LEU:HA	3:SA:54:THR:HG22	2.00	0.44
4:SB:175:GLU:HG3	4:SB:193:ILE:HG12	1.99	0.44
5:SD:177:LEU:O	5:SD:179:GLN:N	2.51	0.44
7:SF:104:THR:HG23	7:SF:106:GLU:HB3	1.99	0.44
23:Sg:116:ASP:HB2	23:Sg:118:ARG:NH2	2.33	0.44
26:SJ:35:TYR:HD2	26:SJ:112:THR:HG21	1.82	0.44
30:SW:66:THR:HG23	30:SW:68:ARG:HB2	2.00	0.44
39:3A:304:ARG:O	39:3A:308:LYS:NZ	2.39	0.44
2:S2:199:C:O2'	2:S2:201:C:OP2	2.36	0.43
2:S2:1240:A:C6	12:SP:100:LYS:HB2	2.53	0.43
4:SB:41:ILE:HG12	4:SB:76:ASN:HB2	1.99	0.43
26:SJ:51:ALA:O	26:SJ:55:LYS:HG2	2.18	0.43
26:SJ:137:VAL:O	26:SJ:140:GLN:N	2.47	0.43
27:SM:79:VAL:HG22	27:SM:80:ASP:H	1.83	0.43
28:SN:100:LYS:HA	28:SN:103:GLU:HG3	2.00	0.43
39:3A:514:MET:HB3	39:3A:517:GLU:HG3	1.98	0.43
39:3A:571:ARG:HA	39:3A:574:THR:HG22	2.00	0.43
42:3E:223:PHE:HB3	42:3E:324:PHE:HB3	2.00	0.43
43:3F:353:LYS:HE3	48:3L:544:ILE:HD12	2.00	0.43
49:3M:46:ILE:HD11	49:3M:86:LEU:HD13	1.98	0.43
49:3M:49:CYS:SG	49:3M:50:ASP:N	2.91	0.43
2:S2:534:G:H2'	2:S2:535:G:C8	2.54	0.43
2:S2:747:U:N3	2:S2:796:G:N1	2.66	0.43
17:SU:28:ASN:HD21	17:SU:31:SER:HB3	1.84	0.43
23:Sg:91:ASP:HB2	23:Sg:98:THR:HG23	2.00	0.43
24:SC:106:VAL:HG22	24:SC:128:VAL:HG22	1.99	0.43
24:SC:246:LYS:HA	24:SC:249:SER:HB3	1.98	0.43
24:SC:278:THR:HA	24:SC:279:ARG:HA	1.71	0.43
40:3B:566:ILE:N	40:3B:580:LEU:O	2.50	0.43
45:3H:69:GLY:HA3	45:3H:78:ILE:HA	1.99	0.43
45:3H:87:HIS:NE2	45:3H:96:GLU:OE1	2.49	0.43
2:S2:906:U:H2'	2:S2:907:G:H8	1.83	0.43
2:S2:906:U:H2'	2:S2:907:G:C8	2.54	0.43
2:S2:1403:C:N4	2:S2:1433:C:OP1	2.48	0.43
2:S2:1775:U:H2'	2:S2:1776:G:C2	2.53	0.43
13:SQ:143:LYS:HE2	13:SQ:145:TYR:HE1	1.83	0.43
29:SO:14:VAL:HG11	29:SO:17:LEU:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:SY:82:ALA:O	31:SY:86:GLU:HB2	2.18	0.43
39:3A:473:ASP:OD1	41:3C:795:TYR:OH	2.28	0.43
39:3A:519:ILE:HG13	39:3A:520:ARG:HD2	1.99	0.43
41:3C:430:ASN:ND2	41:3C:437:PRO:O	2.47	0.43
42:3E:14:LEU:HD21	42:3E:220:PHE:CE2	2.54	0.43
43:3F:93:ARG:HA	43:3F:238:LYS:O	2.18	0.43
45:3H:273:GLN:OE1	45:3H:274:LYS:NZ	2.38	0.43
2:S2:681:U:O2'	2:S2:1160:U:OP1	2.32	0.43
2:S2:1201:U:H2'	2:S2:1202:U:C6	2.54	0.43
2:S2:1777:G:H2'	2:S2:1778:C:H6	1.83	0.43
3:SA:174:MET:HE3	3:SA:174:MET:HB3	1.88	0.43
11:SL:3:ASP:OD1	11:SL:3:ASP:N	2.51	0.43
12:SP:93:MET:HE2	12:SP:93:MET:HB2	1.82	0.43
17:SU:64:THR:HA	17:SU:78:ASP:O	2.19	0.43
19:SX:17:ARG:O	19:SX:21:LYS:HB2	2.19	0.43
24:SC:78:LEU:HB2	24:SC:97:PHE:CD2	2.53	0.43
28:SN:20:ARG:HH21	30:SW:56:HIS:HB3	1.82	0.43
28:SN:36:GLN:HE21	28:SN:36:GLN:HA	1.83	0.43
40:3B:254:LYS:HA	40:3B:260:THR:HA	2.01	0.43
2:S2:1305:C:OP1	35:Sf:93:HIS:NE2	2.52	0.43
4:SB:150:ILE:O	4:SB:151:ARG:HG2	2.18	0.43
6:SE:89:VAL:HG21	6:SE:119:ALA:HA	1.99	0.43
18:SV:27:LYS:HA	18:SV:27:LYS:HD3	1.77	0.43
24:SC:244:ILE:O	24:SC:247:THR:HG22	2.18	0.43
31:SY:11:LYS:O	31:SY:23:MET:HA	2.18	0.43
32:SZ:92:LEU:HD11	32:SZ:109:TYR:CZ	2.53	0.43
40:3B:548:ARG:HB2	40:3B:555:PRO:HD2	2.00	0.43
42:3E:110:GLY:N	42:3E:158:VAL:O	2.50	0.43
2:S2:1309:C:OP1	35:Sf:118:ARG:NH2	2.38	0.43
3:SA:123:VAL:HA	3:SA:145:ILE:O	2.18	0.43
7:SF:121:PRO:HB3	7:SF:196:LEU:HD11	2.00	0.43
20:Sa:13:LYS:HA	20:Sa:13:LYS:HD3	1.77	0.43
20:Sa:19:GLN:HA	20:Sa:20:PRO:HD3	1.86	0.43
34:Se:36:MET:O	34:Se:40:ARG:HB2	2.19	0.43
39:3A:335:ARG:NH2	41:3C:745:LYS:HB3	2.33	0.43
39:3A:347:ILE:O	39:3A:350:GLU:C	2.62	0.43
43:3F:312:VAL:HG11	49:3M:350:LEU:HG	2.00	0.43
49:3M:179:ASP:OD1	49:3M:216:ASN:ND2	2.47	0.43
2:S2:65:C:N4	25:SG:134:GLY:O	2.35	0.43
9:SI:67:TRP:HA	9:SI:189:VAL:HG12	2.01	0.43
9:SI:133:GLU:HA	9:SI:136:ILE:HB	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:SU:37:ALA:O	17:SU:41:ARG:HG3	2.17	0.43
23:Sg:120:ILE:HB	23:Sg:132:TRP:HB2	2.01	0.43
39:3A:340:ARG:HH21	39:3A:345:ASP:HA	1.83	0.43
41:3C:430:ASN:HB3	41:3C:438:LEU:HD12	2.01	0.43
42:3E:414:ARG:HA	42:3E:417:MET:HE2	1.99	0.43
42:3E:422:ILE:HG21	43:3F:354:LEU:HD11	2.01	0.43
47:3K:72:LYS:O	47:3K:75:THR:OG1	2.29	0.43
50:3N:216:PRO:HA	50:3N:464:VAL:HG12	2.01	0.43
2:S2:380:G:N1	2:S2:383:G:OP2	2.44	0.43
2:S2:750:C:N4	2:S2:752:G:OP2	2.51	0.43
3:SA:125:THR:HG22	3:SA:175:TRP:HE1	1.82	0.43
8:SH:129:ILE:HD11	8:SH:180:LEU:HD13	2.00	0.43
12:SP:111:MET:HG2	12:SP:119:PHE:CZ	2.53	0.43
23:Sg:251:ALA:HB2	23:Sg:289:LEU:HD23	2.01	0.43
31:SY:35:VAL:HG13	31:SY:40:ILE:HD11	2.01	0.43
39:3A:371:ILE:HA	39:3A:374:MET:HE2	2.00	0.43
41:3C:611:ARG:NH2	41:3C:675:LEU:O	2.46	0.43
42:3E:372:VAL:HA	42:3E:375:ILE:HG12	1.99	0.43
43:3F:356:ASN:ND2	45:3H:191:ASN:OD1	2.52	0.43
48:3L:333:ILE:HG13	48:3L:334:ARG:HD2	2.01	0.43
2:S2:472:C:O2'	2:S2:474:G:OP1	2.35	0.43
2:S2:1309:C:H4'	35:Sf:133:ALA:HA	2.01	0.43
2:S2:1815:A:H3'	2:S2:1816:G:H8	1.84	0.43
17:SU:18:HIS:HB3	17:SU:117:ALA:HB2	2.01	0.43
26:SJ:134:HIS:ND1	26:SJ:163:SER:HB2	2.34	0.43
34:Se:11:LYS:O	34:Se:15:GLN:HG2	2.19	0.43
39:3A:307:ARG:HD2	39:3A:310:LEU:HB3	2.00	0.43
39:3A:520:ARG:HG3	45:3H:233:LEU:HD12	2.00	0.43
50:3N:341:ASN:HB3	50:3N:344:VAL:HG22	2.00	0.43
2:S2:435:A:OP1	9:SI:23:LYS:NZ	2.50	0.43
2:S2:1146:C:OP1	20:Sa:89:ARG:NH2	2.45	0.43
2:S2:1158:G:H5''	30:SW:76:SER:HB2	2.01	0.43
2:S2:1407:U:H4'	13:SQ:71:ARG:NH2	2.34	0.43
23:Sg:188:HIS:HB3	23:Sg:219:TRP:CZ3	2.51	0.43
42:3E:59:LYS:HA	42:3E:59:LYS:HD3	1.83	0.43
47:3K:143:CYS:HA	47:3K:146:VAL:HG12	2.01	0.43
2:S2:888:U:H2'	2:S2:900:C:H42	1.83	0.42
2:S2:1781:A:H3'	2:S2:1783:C:C4	2.54	0.42
29:SO:44:VAL:HG11	29:SO:85:CYS:SG	2.59	0.42
39:3A:281:THR:HB	39:3A:285:LYS:NZ	2.34	0.42
41:3C:52:ALA:HA	41:3C:55:LYS:HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:3M:109:LEU:O	49:3M:113:MET:HG3	2.19	0.42
2:S2:1222:G:H2'	2:S2:1223:A:C8	2.54	0.42
9:SI:81:VAL:HA	9:SI:102:VAL:HG12	2.01	0.42
11:SL:121:GLN:N	11:SL:124:ASP:OD2	2.43	0.42
12:SP:33:LEU:HD12	12:SP:33:LEU:HA	1.90	0.42
20:Sa:22:ARG:NH1	20:Sa:27:ALA:O	2.50	0.42
25:SG:142:ARG:HE	25:SG:142:ARG:HB3	1.73	0.42
41:3C:835:LEU:HA	41:3C:842:VAL:HA	2.01	0.42
41:3C:837:GLN:HB2	42:3E:348:HIS:HD2	1.83	0.42
47:3K:26:LEU:HA	47:3K:29:LEU:HB2	2.01	0.42
48:3L:369:ALA:O	48:3L:373:ILE:HG23	2.19	0.42
50:3N:261:SER:O	50:3N:515:GLN:NE2	2.45	0.42
2:S2:1010:G:H2'	2:S2:1011:A:C8	2.54	0.42
2:S2:1156:U:OP1	30:SW:71:LYS:NZ	2.50	0.42
5:SD:157:MET:HE2	5:SD:187:LYS:HE3	2.01	0.42
13:SQ:89:SER:HB3	13:SQ:112:LEU:HD13	1.99	0.42
14:SR:128:PHE:CD2	14:SR:129:LYS:HG3	2.54	0.42
23:Sg:114:SER:HB3	23:Sg:119:GLN:HB2	2.00	0.42
39:3A:594:LEU:HD22	39:3A:597:ARG:HH21	1.84	0.42
47:3K:48:LEU:HD12	48:3L:292:LYS:HB3	2.02	0.42
49:3M:213:LYS:HD2	49:3M:213:LYS:HA	1.70	0.42
2:S2:86:C:O2'	2:S2:171:A:N1	2.50	0.42
2:S2:656:G:H21	2:S2:663:C:H5''	1.85	0.42
3:SA:77:ILE:HG12	3:SA:99:ILE:HB	2.01	0.42
19:SX:77:ASN:O	19:SX:79:LYS:N	2.52	0.42
23:Sg:132:TRP:HD1	23:Sg:138:CYS:HA	1.85	0.42
25:SG:116:LYS:HE3	25:SG:116:LYS:HB3	1.78	0.42
47:3K:157:LEU:HA	47:3K:160:GLU:HG3	2.01	0.42
2:S2:67:C:H42	25:SG:167:LYS:HB3	1.85	0.42
2:S2:988:C:O2'	4:SB:118:GLN:O	2.37	0.42
15:SS:67:VAL:HA	15:SS:70:ILE:HG22	2.00	0.42
18:SV:66:ASP:OD1	18:SV:67:ASP:N	2.53	0.42
18:SV:80:SER:HB3	18:SV:83:PHE:HB3	2.02	0.42
25:SG:67:VAL:HB	25:SG:99:GLY:HA2	2.00	0.42
39:3A:269:PRO:HA	39:3A:272:MET:HE2	2.02	0.42
39:3A:406:ARG:O	39:3A:409:LYS:HG3	2.19	0.42
41:3C:455:PHE:CE1	41:3C:459:MET:HE1	2.54	0.42
41:3C:785:GLU:OE1	41:3C:789:ARG:NH1	2.29	0.42
41:3C:870:ASN:HA	41:3C:873:VAL:HG22	2.00	0.42
42:3E:136:LYS:NZ	50:3N:15:GLY:O	2.51	0.42
48:3L:356:LYS:HD2	48:3L:356:LYS:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:SE:19:MET:SD	6:SE:108:ARG:HD2	2.59	0.42
12:SP:85:ILE:HA	12:SP:89:MET:HE2	2.02	0.42
27:SM:95:ASP:OD1	27:SM:95:ASP:N	2.53	0.42
31:SY:129:LYS:HA	31:SY:129:LYS:HD3	1.78	0.42
33:Sb:31:TYR:OH	33:Sb:70:LYS:NZ	2.47	0.42
41:3C:402:LEU:O	41:3C:406:ASN:ND2	2.52	0.42
41:3C:868:GLU:OE1	41:3C:872:ARG:NH1	2.53	0.42
42:3E:176:GLU:HA	42:3E:179:MET:SD	2.59	0.42
43:3F:345:GLN:NE2	45:3H:327:CYS:SG	2.93	0.42
2:S2:14:C:H5'	24:SC:190:SER:OG	2.19	0.42
2:S2:1337:C:P	22:Sd:44:ARG:HH22	2.43	0.42
7:SF:91:ARG:HD2	32:SZ:103:HIS:CE1	2.55	0.42
12:SP:36:LEU:HD23	12:SP:36:LEU:HA	1.93	0.42
22:Sd:30:LEU:HA	22:Sd:39:CYS:HA	2.01	0.42
26:SJ:44:TRP:HA	26:SJ:47:LYS:HG2	2.00	0.42
28:SN:99:ARG:NH2	28:SN:119:GLU:OE2	2.43	0.42
39:3A:268:LYS:HB3	39:3A:271:LEU:HG	2.02	0.42
39:3A:321:ARG:HA	39:3A:424:LEU:HD21	2.02	0.42
43:3F:335:LEU:O	43:3F:338:THR:OG1	2.32	0.42
4:SB:73:ASP:CG	29:SO:128:ARG:HH21	2.27	0.42
5:SD:87:TYR:CD1	44:3G:307:HIS:HA	2.55	0.42
14:SR:26:ASN:O	14:SR:26:ASN:ND2	2.45	0.42
15:SS:47:LYS:HD3	15:SS:47:LYS:HA	1.86	0.42
26:SJ:121:LYS:H	26:SJ:125:HIS:HD2	1.66	0.42
29:SO:14:VAL:H	29:SO:15:ILE:HA	1.84	0.42
31:SY:39:GLU:HA	31:SY:42:GLU:HG2	2.01	0.42
39:3A:291:PHE:O	39:3A:295:THR:HG23	2.20	0.42
41:3C:400:LYS:HE3	41:3C:400:LYS:HB2	1.80	0.42
2:S2:78:C:H1'	25:SG:175:LYS:HG3	2.01	0.42
2:S2:1253:A:H4'	2:S2:1254:C:H5''	2.01	0.42
2:S2:1528:G:O2'	2:S2:1666:C:OP1	2.36	0.42
2:S2:1615:U:O4	12:SP:40:ARG:NH1	2.53	0.42
5:SD:95:GLY:HA2	5:SD:101:GLN:NE2	2.35	0.42
16:ST:3:GLY:HA2	16:ST:4:VAL:HA	1.89	0.42
26:SJ:120:ALA:HB1	26:SJ:125:HIS:CD2	2.55	0.42
30:SW:42:MET:HE2	30:SW:42:MET:HB3	1.79	0.42
41:3C:56:ARG:NH1	41:3C:92:LYS:O	2.53	0.42
41:3C:562:ASP:HB2	50:3N:71:TYR:HD1	1.84	0.42
42:3E:309:GLN:OE1	42:3E:313:ARG:NH2	2.53	0.42
47:3K:171:LYS:HD2	47:3K:171:LYS:HA	1.77	0.42
48:3L:225:HIS:O	48:3L:229:ASN:ND2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:3N:425:LEU:HA	50:3N:432:LEU:HD21	2.02	0.42
18:SV:73:ALA:HB1	18:SV:78:ILE:HB	2.01	0.42
20:Sa:87:ARG:NH1	20:Sa:91:ALA:O	2.53	0.42
22:Sd:15:GLY:C	22:Sd:17:GLY:H	2.28	0.42
25:SG:2:LYS:HB3	25:SG:15:LEU:HD11	2.00	0.42
26:SJ:33:GLY:HA3	34:Se:38:TYR:CG	2.54	0.42
42:3E:369:ARG:HH22	48:3L:477:GLY:HA2	1.84	0.42
42:3E:417:MET:O	42:3E:421:ASN:ND2	2.53	0.42
50:3N:242:GLN:HE21	50:3N:362:ARG:NH2	2.18	0.42
2:S2:1471:C:H42	2:S2:1476:A:N6	2.18	0.41
2:S2:1598:G:H5''	32:SZ:80:ARG:HD3	2.02	0.41
5:SD:170:THR:HG22	5:SD:187:LYS:HG2	2.02	0.41
15:SS:114:LEU:HA	15:SS:117:ILE:HG22	2.02	0.41
17:SU:34:LYS:HE3	17:SU:107:GLU:HG2	2.01	0.41
23:Sg:37:ASP:N	23:Sg:37:ASP:OD1	2.45	0.41
23:Sg:228:TYR:CE2	23:Sg:264:LYS:HG2	2.55	0.41
35:Sf:141:CYS:HB3	35:Sf:146:LEU:HB3	2.02	0.41
39:3A:101:THR:HG22	39:3A:149:TRP:HB3	2.02	0.41
39:3A:350:GLU:C	39:3A:352:GLN:H	2.28	0.41
40:3B:360:TRP:HA	40:3B:367:GLN:HA	2.02	0.41
41:3C:431:LEU:HG	41:3C:432:HIS:CD2	2.55	0.41
47:3K:18:ILE:HD12	48:3L:262:ARG:HH11	1.85	0.41
48:3L:324:LEU:HD11	48:3L:370:LEU:HB3	2.02	0.41
49:3M:185:MET:SD	49:3M:188:LEU:HD22	2.60	0.41
49:3M:344:LYS:HD3	49:3M:344:LYS:HA	1.82	0.41
50:3N:57:ASN:O	50:3N:60:SER:OG	2.34	0.41
2:S2:57:U:O2'	2:S2:499:G:N3	2.50	0.41
2:S2:581:U:H4'	31:SY:66:GLY:HA2	2.02	0.41
2:S2:1551:U:OP2	2:S2:1579:A:N6	2.53	0.41
2:S2:1777:G:H2'	2:S2:1778:C:C6	2.54	0.41
4:SB:33:VAL:HG12	4:SB:96:CYS:HB2	2.01	0.41
4:SB:49:VAL:HB	4:SB:62:LEU:HD21	2.02	0.41
9:SI:94:LYS:HE2	9:SI:94:LYS:HB2	1.82	0.41
12:SP:16:THR:OG1	12:SP:17:TYR:N	2.53	0.41
17:SU:19:ARG:HA	17:SU:91:LEU:O	2.19	0.41
34:Se:28:LYS:HD3	34:Se:32:ALA:HB1	2.01	0.41
42:3E:366:GLU:HA	42:3E:369:ARG:HB2	2.03	0.41
45:3H:233:LEU:HD23	45:3H:340:LYS:HB3	2.02	0.41
45:3H:315:ASP:OD1	45:3H:315:ASP:N	2.53	0.41
48:3L:537:ARG:HH21	48:3L:538:ARG:NH1	2.18	0.41
49:3M:243:ILE:HA	49:3M:247:ALA:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:3N:172:GLU:HG2	50:3N:519:VAL:HG12	2.01	0.41
1:Ln:2:ARG:HD3	1:Ln:5:TRP:NE1	2.35	0.41
2:S2:24:C:O2'	2:S2:25:A:O5'	2.38	0.41
2:S2:375:U:H1'	11:SL:7:GLU:OE2	2.20	0.41
2:S2:587:A:OP2	26:SJ:172:ARG:NH2	2.53	0.41
2:S2:811:A:H2'	2:S2:812:A:C8	2.56	0.41
7:SF:44:LYS:HD2	7:SF:44:LYS:HA	1.77	0.41
11:SL:29:GLY:HA3	11:SL:30:LYS:HA	1.62	0.41
16:ST:6:VAL:HG12	16:ST:135:ALA:HB2	2.01	0.41
20:Sa:75:VAL:O	20:Sa:79:ILE:HG12	2.21	0.41
41:3C:397:MET:HE3	41:3C:397:MET:HB2	1.82	0.41
41:3C:458:ILE:O	41:3C:462:THR:OG1	2.32	0.41
42:3E:20:PHE:HA	42:3E:23:LEU:HB2	2.03	0.41
43:3F:313:ASN:HB2	49:3M:336:HIS:HB2	2.01	0.41
49:3M:239:ASP:OD1	49:3M:240:LEU:N	2.52	0.41
1:Ln:9:ARG:HE	1:Ln:9:ARG:HB3	1.74	0.41
2:S2:1037:G:H4'	2:S2:1845:A:H4'	2.02	0.41
2:S2:1337:C:H4'	17:SU:67:LYS:O	2.21	0.41
4:SB:145:LYS:NZ	14:SR:135:VAL:O	2.33	0.41
7:SF:127:ARG:HB3	7:SF:136:ARG:HB2	2.02	0.41
8:SH:72:PHE:O	8:SH:75:ILE:O	2.37	0.41
9:SI:160:SER:OG	9:SI:161:LEU:N	2.53	0.41
32:SZ:77:LEU:C	32:SZ:78:LYS:HD3	2.45	0.41
41:3C:463:ASP:HA	41:3C:464:PRO:HD3	1.97	0.41
41:3C:671:VAL:HG23	41:3C:676:HIS:CD2	2.56	0.41
42:3E:262:ILE:HG12	42:3E:335:ASN:HB3	2.03	0.41
2:S2:56:G:OP1	31:SY:111:LYS:NZ	2.50	0.41
2:S2:1226:G:N1	2:S2:1639:G:OP2	2.50	0.41
2:S2:1268:C:O2'	12:SP:97:TYR:OH	2.32	0.41
2:S2:1595:U:H2'	2:S2:1596:U:C6	2.55	0.41
4:SB:152:LYS:HE2	4:SB:152:LYS:HB3	1.83	0.41
8:SH:6:ALA:HB2	8:SH:28:LEU:HD22	2.01	0.41
9:SI:139:LYS:HB2	9:SI:141:ARG:HE	1.85	0.41
12:SP:72:LYS:H	12:SP:72:LYS:HD2	1.85	0.41
20:Sa:52:ASP:OD1	20:Sa:52:ASP:N	2.53	0.41
41:3C:515:ASP:OD1	41:3C:579:HIS:NE2	2.50	0.41
41:3C:822:ILE:HA	41:3C:825:MET:SD	2.61	0.41
42:3E:99:GLU:OE2	42:3E:116:TYR:OH	2.37	0.41
42:3E:173:LEU:HD11	42:3E:192:LEU:HD22	2.03	0.41
47:3K:8:ARG:NH2	47:3K:42:TYR:O	2.43	0.41
48:3L:243:GLN:HA	48:3L:246:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:3L:329:TYR:HA	48:3L:332:ALA:HB3	2.01	0.41
50:3N:413:LEU:HB2	50:3N:417:ARG:HH11	1.83	0.41
2:S2:989:C:OP2	4:SB:155:TYR:OH	2.36	0.41
2:S2:1115:U:H3	2:S2:1118:C:N4	2.17	0.41
2:S2:1748:G:H1	2:S2:1786:U:H3	1.67	0.41
23:Sg:116:ASP:HB2	23:Sg:118:ARG:HH21	1.85	0.41
27:SM:71:GLU:HG2	35:Sf:114:ILE:HG23	2.02	0.41
33:Sb:75:GLU:HG2	41:3C:388:ASN:ND2	2.35	0.41
35:Sf:124:ASP:N	35:Sf:124:ASP:OD1	2.53	0.41
44:3G:241:ILE:HD12	44:3G:297:ILE:HD11	2.03	0.41
45:3H:156:LYS:HA	45:3H:159:GLN:HG3	2.02	0.41
2:S2:639:C:H2'	2:S2:640:A:C8	2.56	0.41
2:S2:674:C:H2'	2:S2:675:U:C6	2.56	0.41
2:S2:1113:A:H2'	2:S2:1114:U:C6	2.56	0.41
2:S2:1540:G:OP1	16:ST:39:LEU:HD23	2.20	0.41
3:SA:222:VAL:HG13	3:SA:223:THR:HG23	2.03	0.41
4:SB:222:LYS:NZ	4:SB:223:PHE:O	2.45	0.41
6:SE:114:ILE:HB	6:SE:118:GLU:HB3	2.02	0.41
8:SH:113:LYS:HD2	8:SH:113:LYS:HA	1.91	0.41
17:SU:24:LEU:HD13	17:SU:112:VAL:HG22	2.03	0.41
17:SU:32:LEU:HD23	17:SU:87:ARG:HD2	2.02	0.41
25:SG:64:LYS:HB2	25:SG:97:VAL:HG11	2.01	0.41
26:SJ:111:GLN:HE21	26:SJ:123:ILE:HG12	1.86	0.41
28:SN:115:LEU:O	28:SN:119:GLU:HG2	2.21	0.41
31:SY:55:ILE:HG23	31:SY:75:ILE:HG13	2.03	0.41
33:Sb:70:LYS:HB3	33:Sb:70:LYS:HE2	1.68	0.41
43:3F:93:ARG:HB3	43:3F:238:LYS:HZ3	1.85	0.41
43:3F:98:ILE:O	43:3F:102:ILE:HG12	2.20	0.41
43:3F:139:HIS:CE1	43:3F:141:GLU:HB2	2.55	0.41
49:3M:117:THR:HG23	49:3M:120:ARG:N	2.33	0.41
49:3M:296:THR:HA	49:3M:299:GLN:HG3	2.03	0.41
2:S2:107:A:H2'	2:S2:108:G:C8	2.56	0.41
2:S2:746:C:O2'	2:S2:798:G:N1	2.51	0.41
2:S2:1232:U:H3	2:S2:1526:G:H1	1.69	0.41
3:SA:89:LYS:HD3	14:SR:81:ARG:HH22	1.86	0.41
5:SD:215:ASP:OD1	5:SD:215:ASP:N	2.53	0.41
7:SF:60:ARG:HH21	21:Sc:49:PRO:HB3	1.86	0.41
10:SK:65:ARG:NE	22:Sd:25:SER:HB2	2.35	0.41
13:SQ:40:GLU:OE1	13:SQ:40:GLU:N	2.53	0.41
21:Sc:13:ARG:NH2	50:3N:423:THR:HA	2.32	0.41
23:Sg:104:HIS:CE1	23:Sg:124:SER:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:3C:324:ILE:HB	41:3C:328:VAL:HG11	2.02	0.41
50:3N:264:SER:HB3	50:3N:512:PRO:HB3	2.02	0.41
2:S2:839:C:H41	31:SY:10:ARG:HA	1.86	0.41
2:S2:844:U:H2'	2:S2:845:G:H8	1.85	0.41
2:S2:1189:A:H2'	2:S2:1190:A:H8	1.85	0.41
2:S2:1432:U:H4'	2:S2:1437:C:C2	2.56	0.41
8:SH:31:GLU:O	8:SH:37:LYS:HE2	2.21	0.41
10:SK:90:VAL:O	10:SK:95:ARG:NE	2.54	0.41
11:SL:93:LEU:HG	11:SL:102:PHE:HB3	2.02	0.41
14:SR:27:ASP:O	14:SR:31:ASN:ND2	2.30	0.41
17:SU:95:SER:HA	17:SU:98:VAL:HG22	2.03	0.41
23:Sg:206:LEU:HD11	23:Sg:218:LEU:HD13	2.01	0.41
23:Sg:292:SER:OG	23:Sg:294:ASP:OD1	2.31	0.41
25:SG:231:ARG:O	25:SG:235:SER:OG	2.31	0.41
27:SM:25:ALA:HA	27:SM:28:HIS:CE1	2.56	0.41
29:SO:14:VAL:N	29:SO:15:ILE:HA	2.36	0.41
32:SZ:67:LEU:HD23	32:SZ:67:LEU:HA	1.91	0.41
39:3A:53:LYS:HA	39:3A:53:LYS:HD3	1.88	0.41
39:3A:237:LEU:HD11	39:3A:253:VAL:HG13	2.03	0.41
40:3B:548:ARG:HD3	40:3B:555:PRO:HB2	2.01	0.41
42:3E:121:HIS:CD2	42:3E:124:ARG:HH12	2.39	0.41
42:3E:278:VAL:HA	42:3E:281:ILE:HG22	2.03	0.41
48:3L:438:GLU:HA	48:3L:441:LEU:HG	2.03	0.41
48:3L:487:ARG:HA	48:3L:488:ILE:HA	1.72	0.41
49:3M:286:ALA:HA	49:3M:292:ILE:HD11	2.03	0.41
2:S2:51:U:H2'	2:S2:52:G:C8	2.55	0.41
2:S2:921:G:N1	30:SW:28:ARG:HD2	2.36	0.41
2:S2:1259:A:H1'	2:S2:1264:C:N4	2.36	0.41
12:SP:49:LEU:HD23	12:SP:53:GLN:HG3	2.03	0.41
16:ST:73:GLY:HA2	16:ST:76:THR:HG22	2.03	0.41
23:Sg:29:ASP:O	23:Sg:44:LYS:HA	2.21	0.41
25:SG:223:LYS:HD2	25:SG:223:LYS:HA	1.89	0.41
27:SM:112:LYS:HE2	27:SM:112:LYS:HB2	1.91	0.41
34:Se:27:LYS:HD3	34:Se:27:LYS:HA	1.77	0.41
41:3C:349:ALA:HA	41:3C:352:GLU:HG2	2.03	0.41
45:3H:172:LYS:HD2	45:3H:192:ILE:HD12	2.02	0.41
49:3M:165:LEU:HD12	49:3M:168:LEU:HD12	2.02	0.41
50:3N:61:SER:OG	50:3N:62:GLN:N	2.54	0.41
2:S2:60:A:N3	2:S2:316:G:O2'	2.51	0.40
2:S2:654:A:OP2	2:S2:655:A:O2'	2.27	0.40
2:S2:1284:A:O2'	27:SM:106:CYS:SG	2.66	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:SK:15:LEU:HD21	10:SK:71:LEU:HD13	2.03	0.40
11:SL:154:GLN:NE2	28:SN:135:LEU:O	2.50	0.40
12:SP:111:MET:HA	15:SS:117:ILE:HD11	2.02	0.40
13:SQ:45:ARG:HD3	13:SQ:45:ARG:HA	1.79	0.40
13:SQ:96:TYR:HA	13:SQ:100:VAL:HG22	2.01	0.40
16:ST:11:GLN:H	16:ST:11:GLN:CD	2.30	0.40
20:Sa:10:ARG:HB2	20:Sa:33:ASP:OD2	2.20	0.40
25:SG:41:LEU:HD12	25:SG:41:LEU:HA	1.87	0.40
25:SG:135:PRO:HB2	25:SG:141:ILE:HD13	2.02	0.40
39:3A:417:GLN:HB2	39:3A:420:LYS:HB3	2.03	0.40
45:3H:41:ILE:HD11	45:3H:45:VAL:HG11	2.02	0.40
48:3L:322:ALA:O	48:3L:326:MET:HG3	2.21	0.40
49:3M:78:LYS:HA	49:3M:78:LYS:HD2	1.95	0.40
1:Ln:11:ARG:NH2	2:S2:1184:G:OP1	2.55	0.40
2:S2:150:A:N6	2:S2:169:U:O2	2.54	0.40
2:S2:834:C:H42	2:S2:839:C:H42	1.70	0.40
2:S2:1743:G:H21	2:S2:1791:A:H62	1.69	0.40
7:SF:153:LEU:HD23	7:SF:153:LEU:HA	1.92	0.40
14:SR:114:LEU:HB3	14:SR:115:SER:H	1.57	0.40
19:SX:100:VAL:HG12	19:SX:125:VAL:HA	2.02	0.40
24:SC:176:LYS:HA	24:SC:176:LYS:HD3	1.76	0.40
25:SG:22:ARG:HH21	25:SG:25:ARG:NH1	2.19	0.40
39:3A:446:ILE:HD13	49:3M:316:VAL:HG21	2.03	0.40
42:3E:408:THR:HG21	43:3F:339:TYR:HE2	1.86	0.40
43:3F:97:VAL:HG11	45:3H:51:LYS:HB2	2.03	0.40
43:3F:247:ILE:HG13	45:3H:227:LYS:HE3	2.03	0.40
45:3H:176:VAL:HA	45:3H:179:GLU:HG2	2.02	0.40
45:3H:319:ILE:O	45:3H:323:ILE:HG12	2.22	0.40
50:3N:237:LYS:HA	50:3N:240:LYS:HG2	2.03	0.40
50:3N:248:THR:HG22	50:3N:374:ARG:HB3	2.02	0.40
50:3N:451:TYR:HE2	50:3N:469:GLN:HB2	1.86	0.40
2:S2:595:U:H2'	2:S2:596:U:C6	2.56	0.40
2:S2:1365:G:H2'	2:S2:1366:G:C8	2.55	0.40
2:S2:1623:A:N7	15:SS:132:ARG:HB3	2.36	0.40
3:SA:70:ASN:HA	3:SA:71:PRO:HD2	1.98	0.40
14:SR:59:LYS:HE3	14:SR:59:LYS:HB2	1.91	0.40
21:Sc:14:VAL:HG12	21:Sc:54:ASP:O	2.21	0.40
23:Sg:99:ARG:HH11	23:Sg:135:LEU:HD22	1.86	0.40
23:Sg:257:LYS:HB2	23:Sg:257:LYS:HE2	1.99	0.40
25:SG:102:VAL:HG21	25:SG:109:LEU:HD21	2.03	0.40
27:SM:18:LEU:HD22	27:SM:77:ILE:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:3A:326:THR:HA	39:3A:329:ILE:HG13	2.04	0.40
39:3A:414:VAL:O	39:3A:425:GLN:NE2	2.37	0.40
41:3C:70:ALA:HA	41:3C:73:ILE:HG12	2.03	0.40
41:3C:856:ALA:HA	41:3C:859:LEU:HD12	2.02	0.40
45:3H:67:LEU:HD23	45:3H:78:ILE:HG13	2.03	0.40
48:3L:239:ASN:OD1	48:3L:242:ARG:NH1	2.55	0.40
48:3L:301:LYS:HE3	48:3L:302:LYS:HD3	2.04	0.40
49:3M:42:LEU:HD13	49:3M:70:LEU:HD11	2.03	0.40
2:S2:582:U:OP1	26:SJ:162:ARG:NH1	2.54	0.40
2:S2:1594:A:H5''	32:SZ:104:ARG:HB3	2.02	0.40
2:S2:1616:U:O4	12:SP:40:ARG:NH1	2.54	0.40
3:SA:9:GLN:HG3	3:SA:10:MET:H	1.85	0.40
7:SF:123:GLU:OE2	21:Sc:63:ARG:NH2	2.54	0.40
9:SI:43:ILE:HA	9:SI:56:ARG:O	2.22	0.40
14:SR:16:ILE:HG22	14:SR:24:LEU:HD11	2.04	0.40
15:SS:124:ARG:O	15:SS:127:TRP:O	2.40	0.40
25:SG:78:SER:OG	25:SG:79:LYS:N	2.53	0.40
39:3A:550:HIS:CE1	45:3H:216:TRP:HB3	2.57	0.40
41:3C:643:LYS:HB3	41:3C:679:LEU:HD21	2.04	0.40
42:3E:88:THR:HG22	42:3E:91:ILE:HD13	2.03	0.40
42:3E:418:LEU:HD11	43:3F:350:LEU:HD22	2.03	0.40
43:3F:265:LEU:N	45:3H:203:ILE:O	2.51	0.40
45:3H:210:LEU:O	45:3H:214:LEU:HD23	2.22	0.40
48:3L:253:PRO:HA	48:3L:256:VAL:HG12	2.02	0.40
2:S2:17:C:H2'	2:S2:18:C:C6	2.57	0.40
2:S2:1177:U:H2'	2:S2:1178:U:C6	2.56	0.40
2:S2:1256:G:C8	17:SU:66:ARG:HB2	2.57	0.40
2:S2:1413:G:H2'	2:S2:1414:A:H8	1.87	0.40
2:S2:1589:A:H2'	2:S2:1590:C:C6	2.57	0.40
4:SB:97:LEU:HB3	4:SB:232:HIS:CD2	2.56	0.40
5:SD:48:ILE:HB	5:SD:86:LEU:HG	2.04	0.40
7:SF:150:ALA:O	7:SF:154:LEU:HG	2.22	0.40
14:SR:67:ARG:HB3	14:SR:68:GLY:H	1.58	0.40
32:SZ:99:LEU:HA	32:SZ:109:TYR:HD1	1.86	0.40
39:3A:129:LEU:HA	39:3A:132:VAL:HG22	2.02	0.40
39:3A:271:LEU:HA	39:3A:274:ASN:HD21	1.87	0.40
39:3A:347:ILE:HG22	39:3A:351:LYS:HE2	2.03	0.40
41:3C:372:VAL:HG13	41:3C:440:VAL:HG11	2.04	0.40
43:3F:150:MET:O	43:3F:154:LYS:HG2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Ln	23/24 (96%)	23 (100%)	0	100	100
3	SA	183/243 (75%)	183 (100%)	0	100	100
4	SB	195/231 (84%)	195 (100%)	0	100	100
5	SD	190/202 (94%)	189 (100%)	1 (0%)	81	80
6	SE	224/225 (100%)	224 (100%)	0	100	100
7	SF	159/170 (94%)	158 (99%)	1 (1%)	78	79
8	SH	166/174 (95%)	166 (100%)	0	100	100
9	SI	178/180 (99%)	177 (99%)	1 (1%)	78	79
10	SK	89/136 (65%)	89 (100%)	0	100	100
11	SL	137/142 (96%)	136 (99%)	1 (1%)	76	78
12	SP	107/130 (82%)	107 (100%)	0	100	100
13	SQ	119/121 (98%)	119 (100%)	0	100	100
14	SR	122/122 (100%)	121 (99%)	1 (1%)	73	77
15	SS	126/132 (96%)	126 (100%)	0	100	100
16	ST	113/115 (98%)	112 (99%)	1 (1%)	70	76
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%)	57 (100%)	0	100	100
22	Sd	48/49 (98%)	48 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	81	80
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%)	129 (99%)	1 (1%)	73	77
29	SO	110/119 (92%)	107 (97%)	3 (3%)	39	61
30	SW	112/113 (99%)	112 (100%)	0	100	100
31	SY	113/115 (98%)	113 (100%)	0	100	100
32	SZ	66/103 (64%)	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	60/140 (43%)	60 (100%)	0	100	100
38	CD	37/404 (9%)	37 (100%)	0	100	100
39	3A	544/1259 (43%)	544 (100%)	0	100	100
40	3B	90/702 (13%)	89 (99%)	1 (1%)	65	74
41	3C	553/811 (68%)	553 (100%)	0	100	100
42	3E	380/406 (94%)	380 (100%)	0	100	100
43	3F	237/289 (82%)	237 (100%)	0	100	100
44	3G	70/277 (25%)	70 (100%)	0	100	100
45	3H	269/310 (87%)	269 (100%)	0	100	100
47	3K	192/193 (100%)	192 (100%)	0	100	100
48	3L	342/515 (66%)	341 (100%)	1 (0%)	86	83
49	3M	304/335 (91%)	304 (100%)	0	100	100
50	3N	398/494 (81%)	398 (100%)	0	100	100
All	All	7658/10679 (72%)	7645 (100%)	13 (0%)	85	85

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	SD	76	ARG
7	SF	36	GLN
9	SI	7	ASN

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Mol	Chain	Res	Type
11	SL	18	GLN
14	SR	26	ASN
16	ST	142	ASN
25	SG	65	GLN
28	SN	36	GLN
29	SO	67	ASP
29	SO	68	GLU
29	SO	105	THR
40	3B	497	GLN
48	3L	407	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95) such sidechains are listed below:

Mol	Chain	Res	Type
1	Ln	22	GLN
3	SA	9	GLN
5	SD	22	ASN
5	SD	179	GLN
6	SE	36	HIS
7	SF	31	ASN
7	SF	203	ASN
8	SH	76	GLN
10	SK	7	ASN
10	SK	66	HIS
10	SK	73	ASN
11	SL	18	GLN
11	SL	19	ASN
12	SP	98	ASN
13	SQ	48	GLN
13	SQ	80	GLN
14	SR	116	ASN
15	SS	10	GLN
15	SS	97	GLN
16	ST	12	GLN
17	SU	47	ASN
17	SU	85	HIS
18	SV	35	ASN
19	SX	16	HIS
19	SX	73	GLN
21	Sc	26	GLN
23	Sg	20	GLN
23	Sg	104	HIS

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Mol	Chain	Res	Type
23	Sg	119	GLN
24	SC	136	HIS
24	SC	267	GLN
24	SC	272	HIS
25	SG	110	ASN
25	SG	155	GLN
26	SJ	154	GLN
28	SN	36	GLN
28	SN	58	HIS
30	SW	24	GLN
30	SW	64	ASN
32	SZ	106	GLN
34	Se	44	ASN
34	Se	58	ASN
35	Sf	91	ASN
39	3A	10	ASN
39	3A	25	GLN
39	3A	110	GLN
39	3A	179	GLN
39	3A	187	GLN
39	3A	229	HIS
39	3A	270	GLN
39	3A	312	GLN
39	3A	430	GLN
39	3A	510	HIS
39	3A	512	GLN
39	3A	588	GLN
41	3C	406	ASN
41	3C	465	HIS
41	3C	519	HIS
41	3C	630	HIS
41	3C	637	GLN
41	3C	828	ASN
41	3C	870	ASN
42	3E	335	ASN
42	3E	349	GLN
43	3F	133	ASN
43	3F	160	HIS
43	3F	271	GLN
44	3G	311	ASN
45	3H	38	GLN
45	3H	58	GLN

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Mol	Chain	Res	Type
45	3H	141	GLN
45	3H	242	ASN
45	3H	266	ASN
45	3H	276	GLN
45	3H	329	ASN
47	3K	57	ASN
47	3K	119	GLN
48	3L	243	GLN
48	3L	296	ASN
48	3L	338	ASN
48	3L	364	ASN
48	3L	368	HIS
48	3L	407	GLN
48	3L	436	HIS
48	3L	499	ASN
49	3M	79	GLN
49	3M	104	GLN
49	3M	108	ASN
49	3M	146	GLN
49	3M	199	GLN
49	3M	238	HIS
49	3M	366	ASN
50	3N	31	GLN
50	3N	385	ASN
50	3N	427	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	S2	1699/1869 (90%)	431 (25%)	4 (0%)

All (431) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	S2	2	A
2	S2	4	C
2	S2	17	C
2	S2	23	G
2	S2	25	A
2	S2	33	G
2	S2	42	A

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Mol	Chain	Res	Type
2	S2	44	U
2	S2	46	A
2	S2	56	G
2	S2	58	C
2	S2	59	U
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	100	U
2	S2	103	A
2	S2	113	G
2	S2	115	U
2	S2	126	G
2	S2	127	C
2	S2	129	C
2	S2	130	G
2	S2	143	U
2	S2	145	G
2	S2	155	G
2	S2	158	A
2	S2	161	U
2	S2	162	C
2	S2	163	U
2	S2	170	A
2	S2	177	G
2	S2	179	C
2	S2	182	C
2	S2	184	G
2	S2	190	G
2	S2	196	C
2	S2	197	U
2	S2	198	U
2	S2	200	G
2	S2	203	G
2	S2	204	G
2	S2	206	G

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Mol	Chain	Res	Type
2	S2	207	G
2	S2	208	G
2	S2	212	C
2	S2	214	U
2	S2	220	U
2	S2	224	A
2	S2	290	U
2	S2	291	G
2	S2	292	A
2	S2	293	C
2	S2	295	C
2	S2	306	C
2	S2	307	G
2	S2	308	G
2	S2	309	G
2	S2	314	U
2	S2	318	A
2	S2	319	C
2	S2	322	C
2	S2	323	C
2	S2	324	C
2	S2	325	C
2	S2	326	C
2	S2	327	G
2	S2	328	U
2	S2	329	G
2	S2	332	G
2	S2	343	A
2	S2	361	U
2	S2	362	C
2	S2	363	A
2	S2	364	A
2	S2	368	U
2	S2	369	C
2	S2	370	G
2	S2	375	U
2	S2	381	C
2	S2	385	G
2	S2	386	C
2	S2	400	C
2	S2	409	C
2	S2	421	G

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Mol	Chain	Res	Type
2	S2	429	C
2	S2	436	G
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	471	G
2	S2	472	C
2	S2	473	A
2	S2	474	G
2	S2	483	C
2	S2	487	U
2	S2	488	U
2	S2	492	C
2	S2	502	C
2	S2	503	C
2	S2	512	A
2	S2	517	C
2	S2	518	G
2	S2	525	A
2	S2	530	U
2	S2	531	A
2	S2	532	C
2	S2	533	A
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	550	C
2	S2	551	U
2	S2	555	A
2	S2	556	U
2	S2	557	U
2	S2	558	G
2	S2	559	G
2	S2	563	G

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Mol	Chain	Res	Type
2	S2	566	U
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	594	A
2	S2	596	U
2	S2	597	G
2	S2	603	C
2	S2	605	A
2	S2	606	G
2	S2	608	C
2	S2	610	G
2	S2	614	C
2	S2	623	G
2	S2	625	G
2	S2	626	G
2	S2	627	U
2	S2	628	A
2	S2	643	A
2	S2	644	G
2	S2	655	A
2	S2	657	U
2	S2	659	G
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	688	U
2	S2	689	U
2	S2	749	U
2	S2	751	G
2	S2	752	G
2	S2	788	G
2	S2	790	C
2	S2	791	C

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Mol	Chain	Res	Type
2	S2	792	C
2	S2	794	A
2	S2	797	C
2	S2	798	G
2	S2	799	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	835	C
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	846	G
2	S2	847	A
2	S2	870	A
2	S2	874	G
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	892	U
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
2	S2	916	A
2	S2	917	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	954	U
2	S2	955	A
2	S2	971	G
2	S2	972	A
2	S2	982	G
2	S2	989	C
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	1033	G
2	S2	1044	G
2	S2	1045	U
2	S2	1057	C
2	S2	1061	U
2	S2	1062	A
2	S2	1076	G
2	S2	1078	C
2	S2	1083	A
2	S2	1085	C
2	S2	1088	U
2	S2	1109	C
2	S2	1114	U
2	S2	1115	U
2	S2	1116	C
2	S2	1118	C
2	S2	1119	A
2	S2	1120	U
2	S2	1121	G
2	S2	1132	C
2	S2	1138	C
2	S2	1140	G
2	S2	1150	A

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Mol	Chain	Res	Type
2	S2	1153	C
2	S2	1154	U
2	S2	1157	G
2	S2	1165	G
2	S2	1170	A
2	S2	1195	A
2	S2	1200	A
2	S2	1203	G
2	S2	1207	G
2	S2	1208	A
2	S2	1215	C
2	S2	1216	C
2	S2	1217	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	1264	C
2	S2	1274	G
2	S2	1275	G
2	S2	1283	C
2	S2	1285	G
2	S2	1286	G
2	S2	1293	A
2	S2	1294	G
2	S2	1295	A
2	S2	1298	G
2	S2	1301	A
2	S2	1302	G
2	S2	1303	C
2	S2	1308	U
2	S2	1313	A
2	S2	1320	G
2	S2	1321	G
2	S2	1331	C
2	S2	1332	A
2	S2	1342	U

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Mol	Chain	Res	Type
2	S2	1348	G
2	S2	1363	C
2	S2	1371	U
2	S2	1372	U
2	S2	1373	C
2	S2	1376	A
2	S2	1378	A
2	S2	1403	C
2	S2	1404	U
2	S2	1417	C
2	S2	1419	C
2	S2	1421	A
2	S2	1422	G
2	S2	1423	C
2	S2	1435	C
2	S2	1436	C
2	S2	1447	G
2	S2	1449	G
2	S2	1450	G
2	S2	1452	A
2	S2	1454	A
2	S2	1463	U
2	S2	1476	A
2	S2	1480	A
2	S2	1486	A
2	S2	1488	C
2	S2	1489	A
2	S2	1490	G
2	S2	1493	C
2	S2	1494	U
2	S2	1495	G
2	S2	1497	G
2	S2	1498	A
2	S2	1508	A
2	S2	1509	U
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	1544	C

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Mol	Chain	Res	Type
2	S2	1552	G
2	S2	1553	C
2	S2	1556	A
2	S2	1563	G
2	S2	1570	G
2	S2	1578	U
2	S2	1580	A
2	S2	1585	U
2	S2	1587	G
2	S2	1588	A
2	S2	1599	U
2	S2	1600	G
2	S2	1601	A
2	S2	1606	G
2	S2	1621	U
2	S2	1623	A
2	S2	1632	G
2	S2	1634	A
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	1679	A
2	S2	1680	G
2	S2	1695	A
2	S2	1696	C
2	S2	1700	C
2	S2	1702	G
2	S2	1709	G
2	S2	1719	A
2	S2	1722	G
2	S2	1723	G
2	S2	1726	G
2	S2	1728	U
2	S2	1729	U
2	S2	1730	U
2	S2	1742	C
2	S2	1743	G
2	S2	1744	G

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Mol	Chain	Res	Type
2	S2	1746	U
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	1760	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	1782	G
2	S2	1783	C
2	S2	1784	G
2	S2	1786	U
2	S2	1787	G
2	S2	1806	A
2	S2	1808	U
2	S2	1809	A
2	S2	1810	U
2	S2	1812	U
2	S2	1813	A
2	S2	1820	G
2	S2	1822	A
2	S2	1823	A
2	S2	1824	A
2	S2	1825	A
2	S2	1826	G
2	S2	1827	U
2	S2	1829	G
2	S2	1831	A
2	S2	1835	A
2	S2	1838	U
2	S2	1848	U
2	S2	1849	G
2	S2	1852	C
2	S2	1861	G

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Mol	Chain	Res	Type
2	S2	1862	G
2	S2	1863	A
2	S2	1864	U
2	S2	1865	C

All (4) RNA pucker outliers are listed below:

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

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 26 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 ⓘ

There are no chain breaks in this entry.

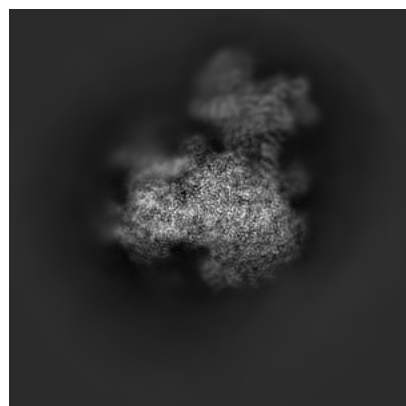
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38754. These allow visual inspection of the internal detail of the map and identification of artifacts.

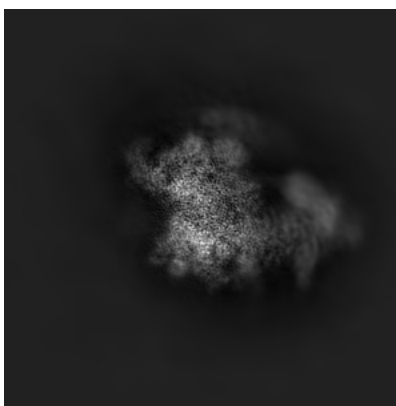
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

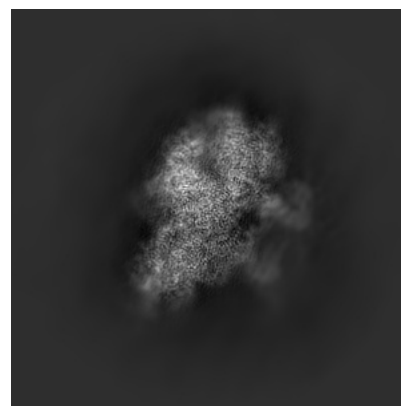
6.1.1 Primary map



X

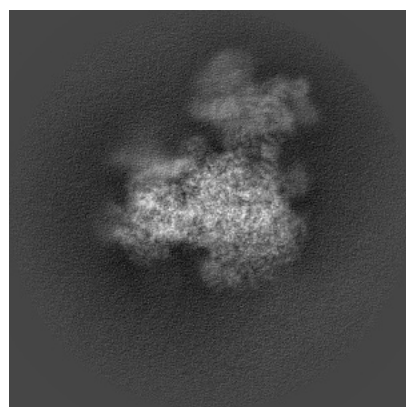


Y

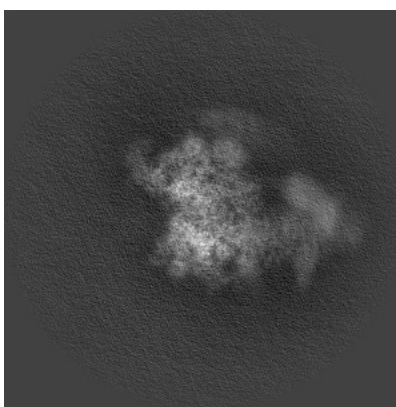


Z

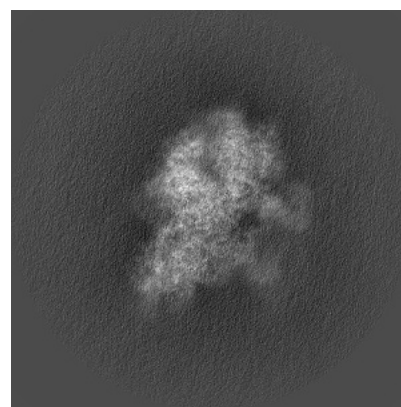
6.1.2 Raw map



X



Y



Z

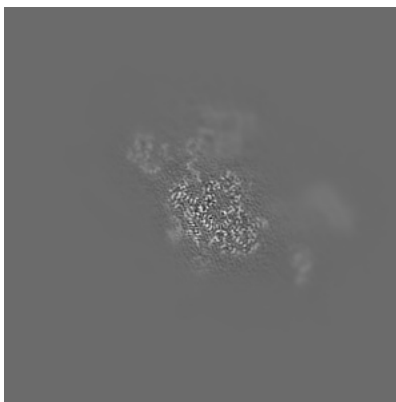
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

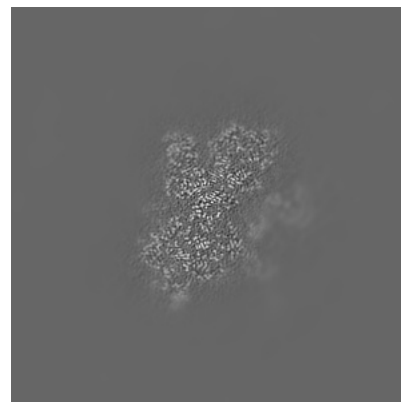
6.2.1 Primary map



X Index: 210

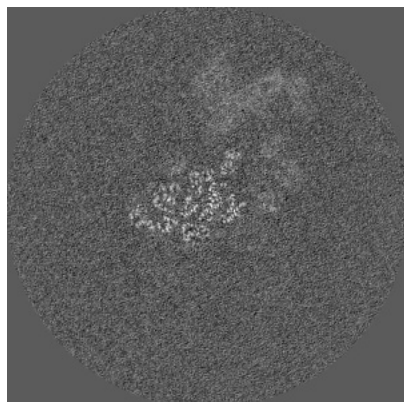


Y Index: 210

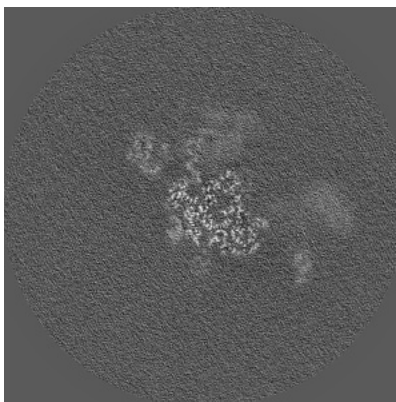


Z Index: 210

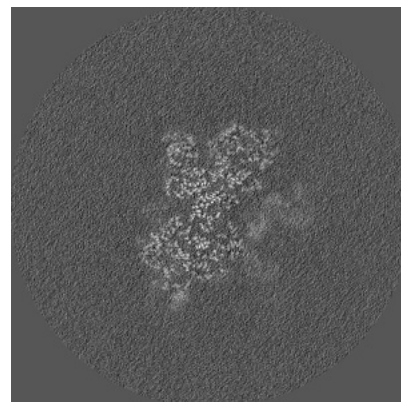
6.2.2 Raw map



X Index: 210



Y Index: 210

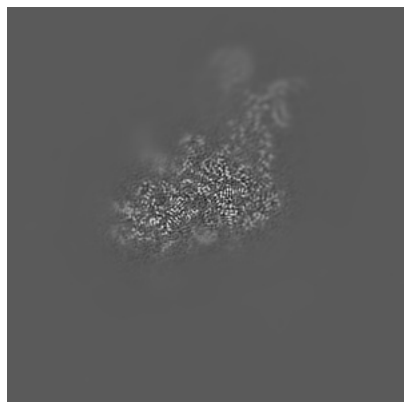


Z Index: 210

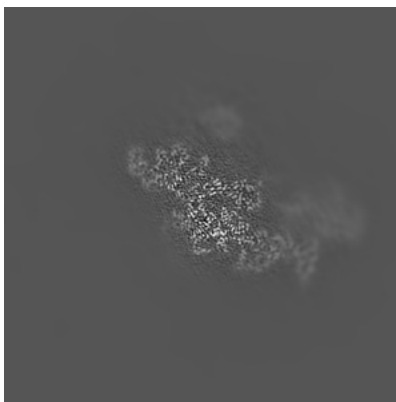
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

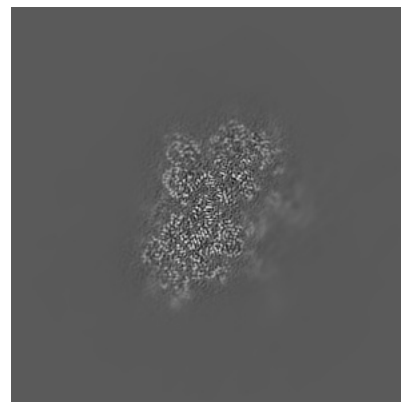
6.3.1 Primary map



X Index: 183

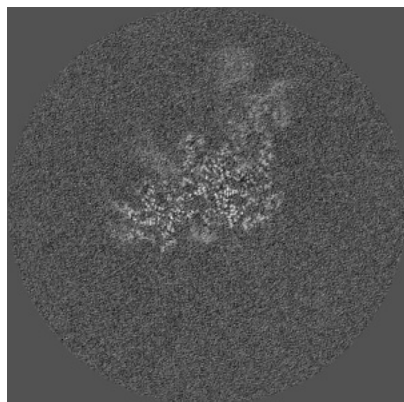


Y Index: 231

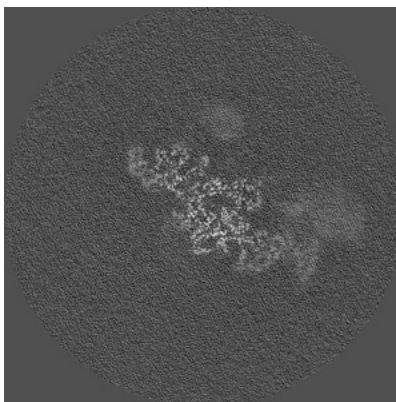


Z Index: 207

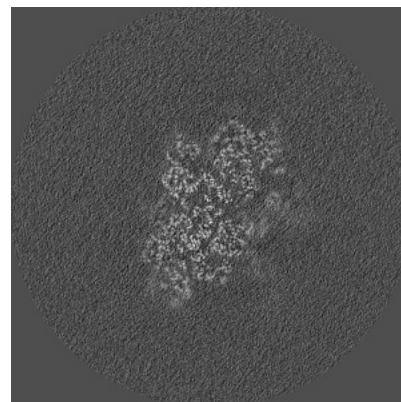
6.3.2 Raw map



X Index: 182



Y Index: 231

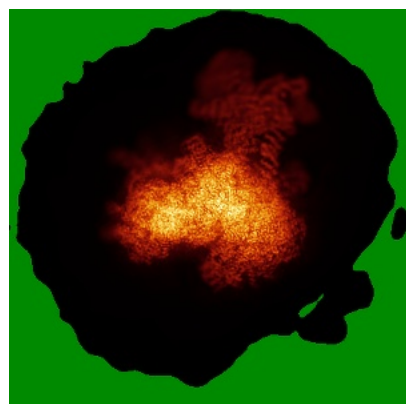


Z Index: 206

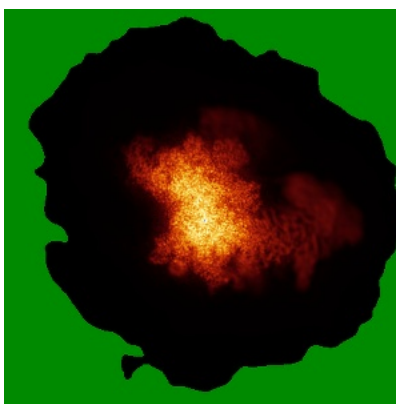
The images above show the largest variance slices of the map in three orthogonal directions.

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

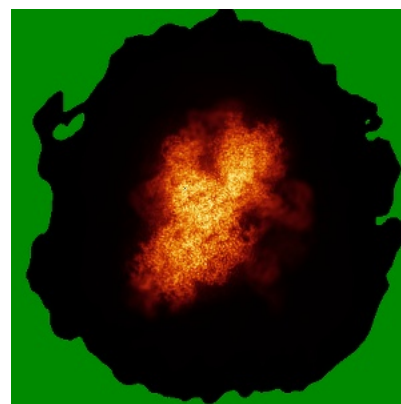
6.4.1 Primary map



X

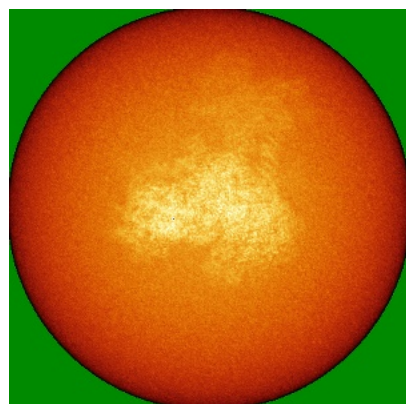


Y

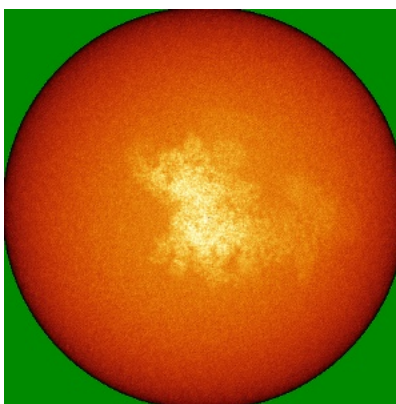


Z

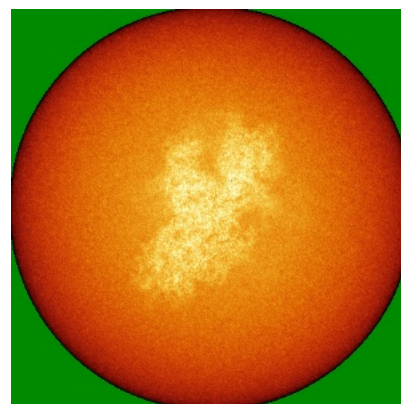
6.4.2 Raw map



X



Y

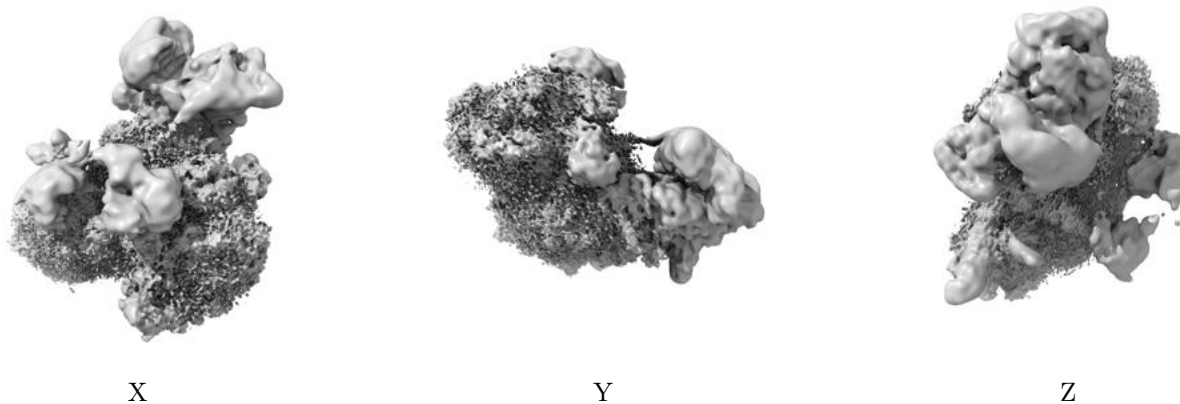


Z

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.

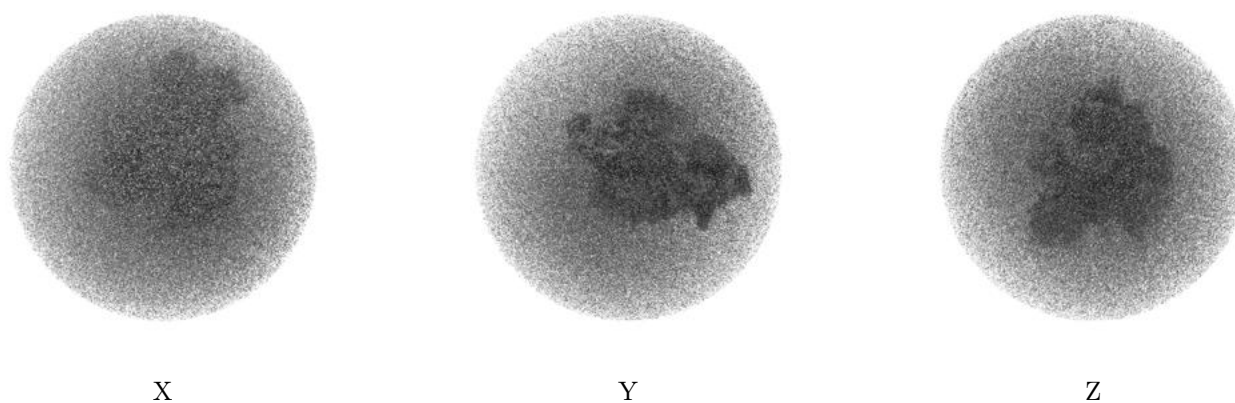
6.5 Orthogonal surface views [i](#)

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.

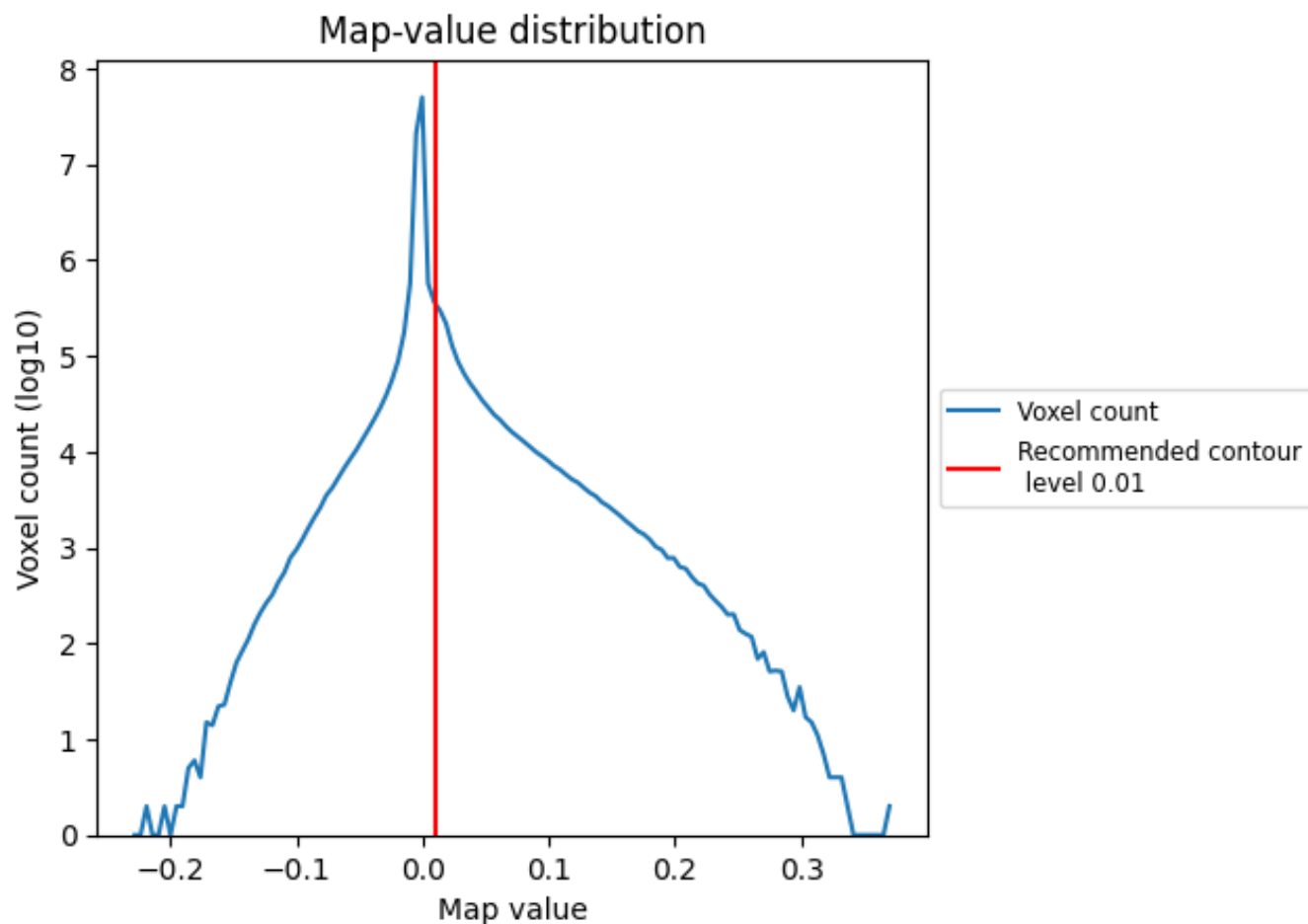
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

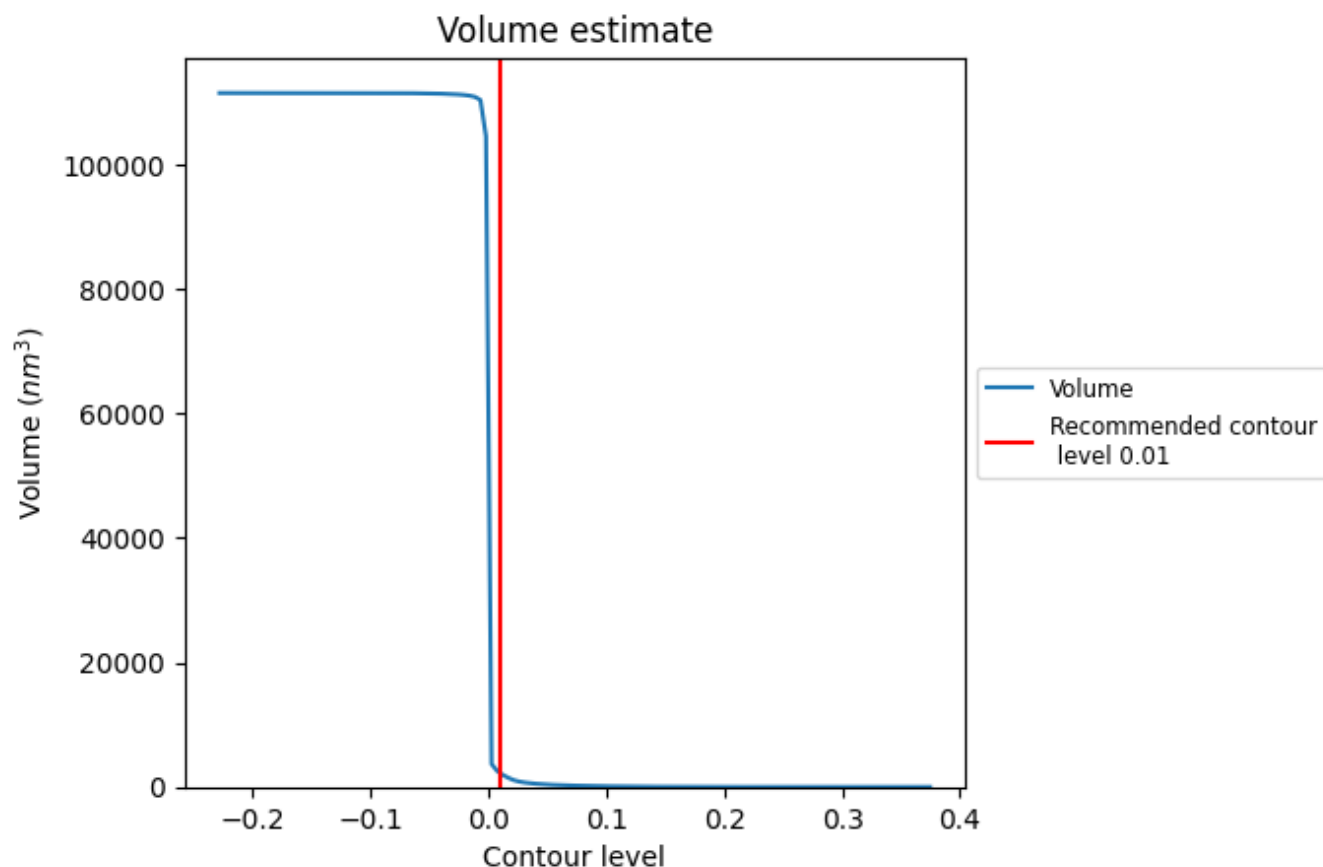
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

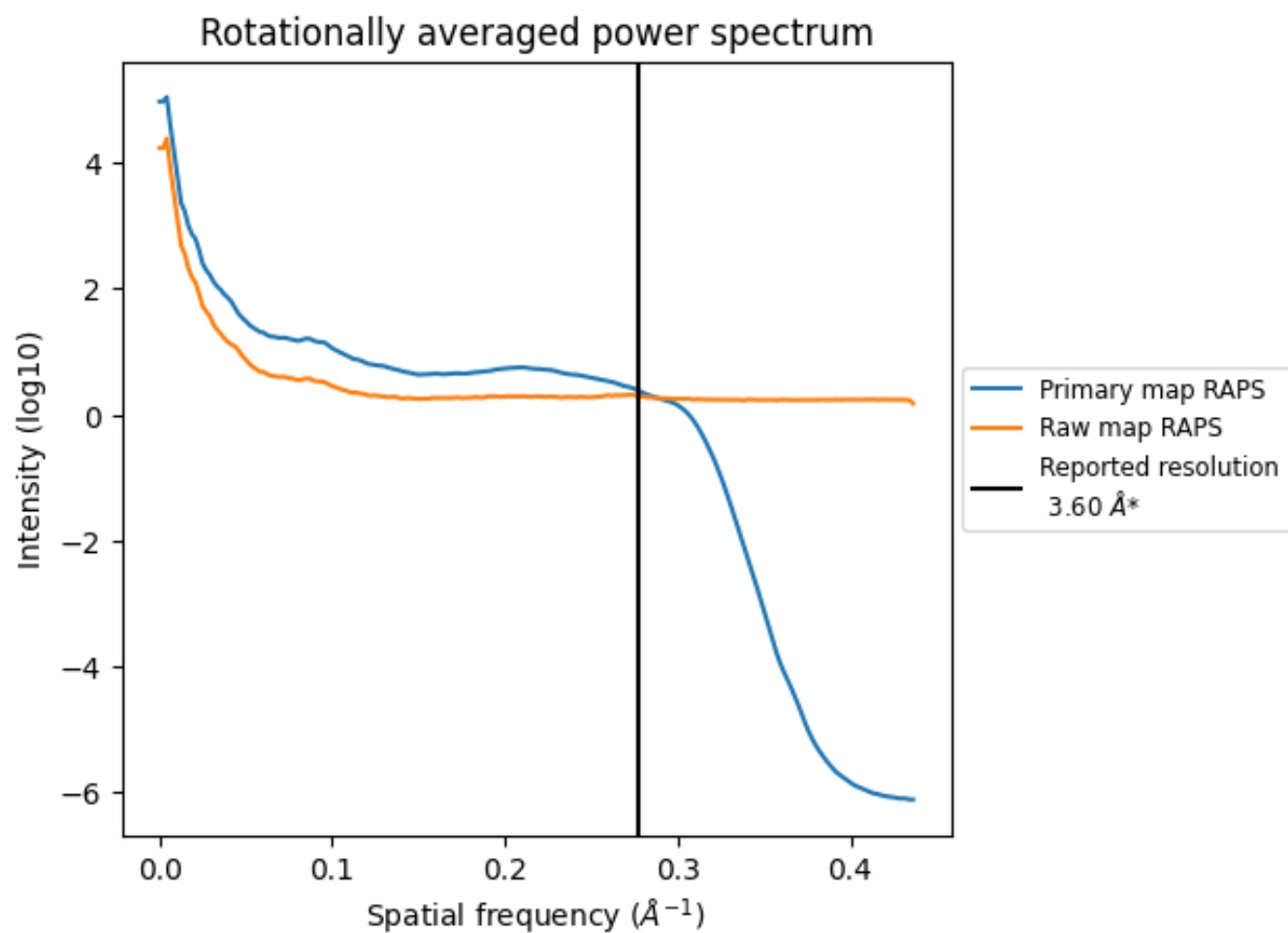
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2214 nm^3 ; this corresponds to an approximate mass of 2000 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 ⓘ

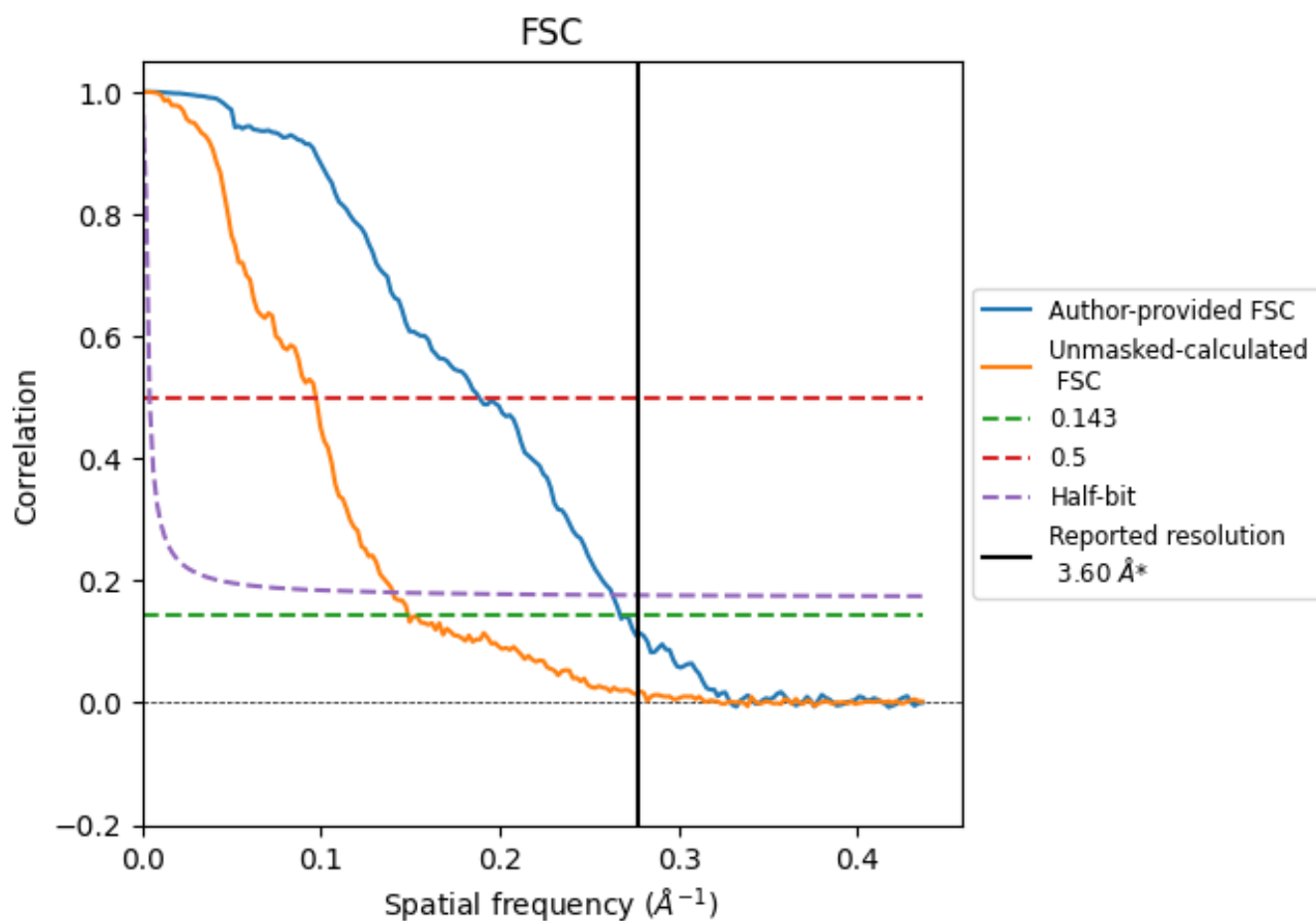


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.278 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.74	5.31	3.80
Unmasked-calculated*	6.72	10.29	7.13

*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 6.72 differs from the reported value 3.6 by more than 10 %

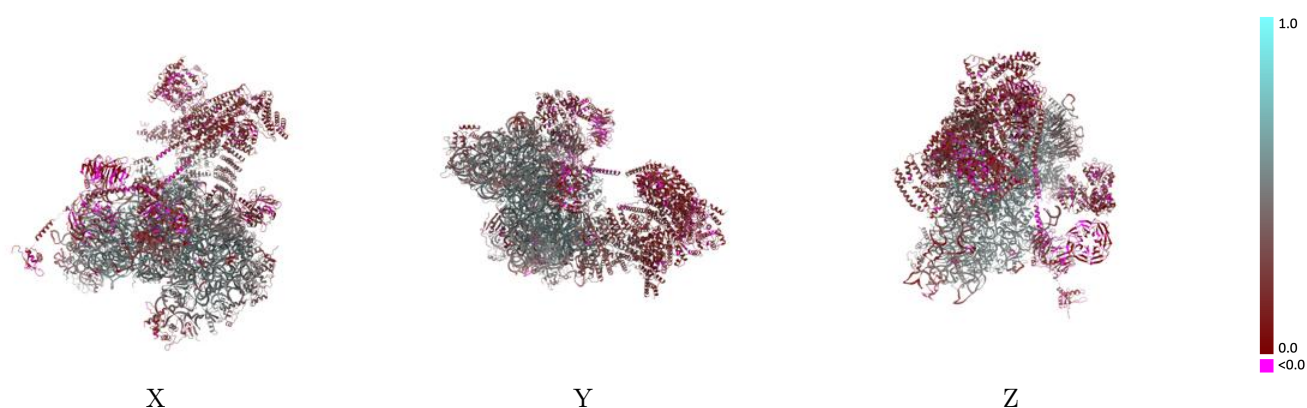
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38754 and PDB model 8XXN. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)

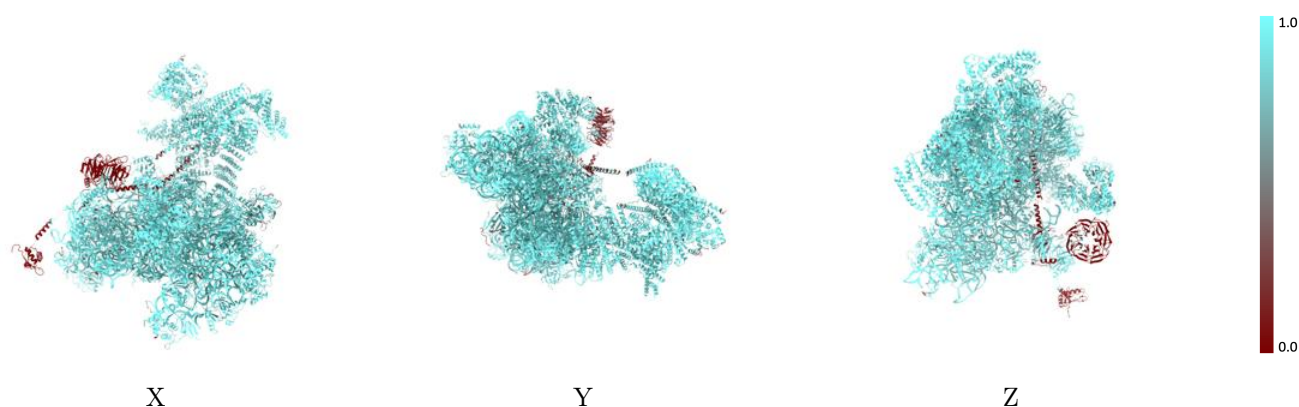
This section was not generated.

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



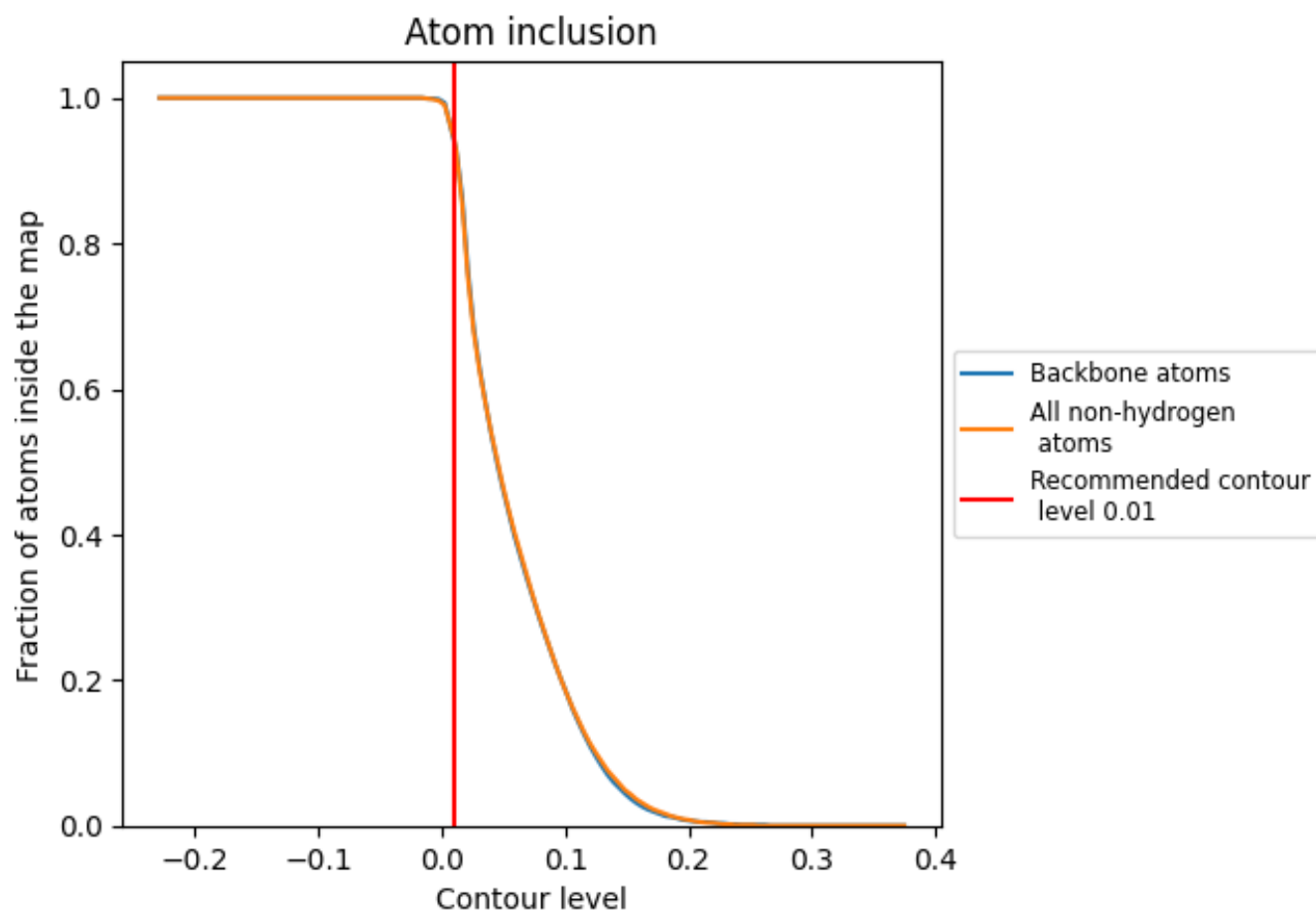
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 94% of all backbone atoms, 94% 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	 0.9450	 0.3740
3A	 0.9040	 0.2270
3B	 0.7020	 0.1290
3C	 0.9470	 0.3030
3E	 0.9700	 0.1700
3F	 0.9620	 0.1150
3G	 0.9830	 0.3040
3H	 0.9600	 0.1330
3I	 0.0760	 0.0340
3K	 0.9530	 0.1120
3L	 0.9440	 0.1020
3M	 0.9870	 0.1520
3N	 0.8220	 0.1860
4A	 0.9480	 0.1480
C1	 0.6820	 0.2590
CD	 0.9670	 0.2320
Ln	 0.8520	 0.3970
S2	 0.9900	 0.4850
SA	 0.9610	 0.4950
SB	 0.9770	 0.4800
SC	 0.9740	 0.5270
SD	 0.9720	 0.4950
SE	 0.9830	 0.5260
SF	 0.9510	 0.4530
SG	 0.9840	 0.4140
SH	 0.9690	 0.4300
SI	 0.9780	 0.4550
SJ	 0.9730	 0.5110
SK	 0.9790	 0.4530
SL	 0.9600	 0.5040
SM	 0.9200	 0.2250
SN	 0.9800	 0.5050
SO	 0.9430	 0.4670
SP	 0.9570	 0.4420
SQ	 0.9600	 0.4990



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Chain	Atom inclusion	Q-score
SR	 0.9500	 0.4640
SS	 0.9470	 0.4140
ST	 0.9690	 0.4540
SU	 0.9640	 0.4310
SV	 0.9840	 0.5070
SW	 0.9810	 0.5560
SX	 0.9800	 0.5370
SY	 0.9560	 0.4710
SZ	 0.9190	 0.3480
Sa	 0.9730	 0.5240
Sb	 0.9560	 0.4980
Sc	 0.9360	 0.4050
Sd	 0.9820	 0.5310
Se	 0.9370	 0.4670
Sf	 0.9480	 0.3020
Sg	 0.9820	 0.3780