



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 10:30 PM UTC

PDB ID : 8EA3 / pdb_00008ea3
EMDB ID : EMD-27971
Title : V-K CAST Transpososome from *Scytonema hofmanni*, major configuration
Authors : Rizo, A.N.; Park, J.-U.; Tsai, A.W.; Kellogg, E.H.
Deposited on : 2022-08-27
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

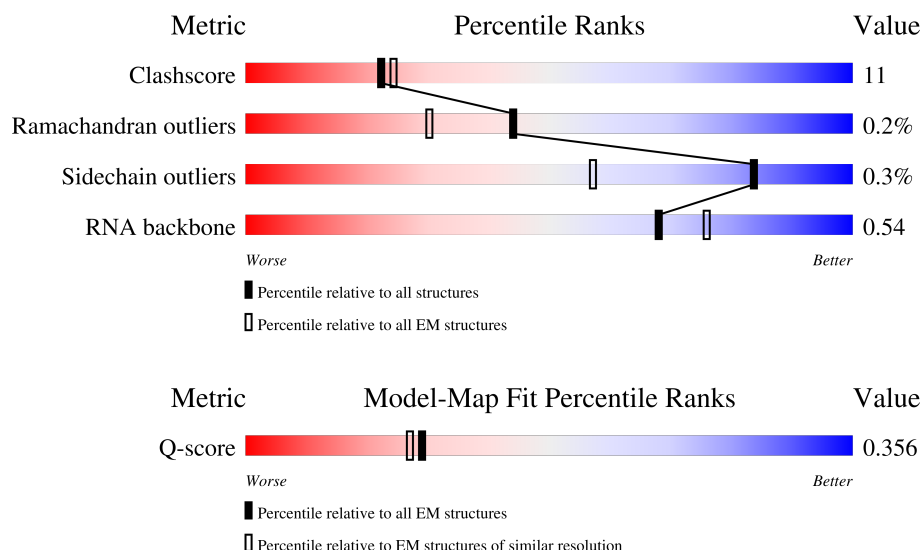
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11569 (3.20 - 4.20)

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	1	141	
2	3	71	
3	7	265	

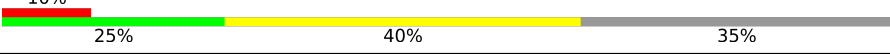
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Mol	Chain	Length	Quality of chain
4	A	276	
4	B	276	
4	C	276	
4	D	276	
4	E	276	
4	F	276	
4	G	276	
4	H	276	
4	I	276	
4	J	276	
4	K	276	
4	L	276	
5	O	639	
6	Q	167	
7	S	89	
8	W	584	
8	X	584	
8	Y	584	
8	Z	584	
8	w	584	
8	x	584	
8	y	584	
8	z	584	
9	2	51	
10	4	75	

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Mol	Chain	Length	Quality of chain
11	5	50	
12	6	20	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	MG	F	301	-	-	X	-
13	MG	G	301	-	-	X	-

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 55955 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 DNA chain called Target_LE.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	99	Total	C	N	O	P	0	0
			2031	971	373	588	99		

- Molecule 2 is a DNA chain called Non-target_R.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	50	Total	C	N	O	P	0	0
			1022	490	179	303	50		

- Molecule 3 is a RNA chain called sg_RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	7	230	Total	C	N	O	P	0	0
			4896	2187	863	1616	230		

- Molecule 4 is a protein called TnsC.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	257	Total	C	N	O	S	0	0
			2066	1306	377	375	8		
4	B	257	Total	C	N	O	S	0	0
			2066	1306	377	375	8		
4	C	257	Total	C	N	O	S	0	0
			2066	1306	377	375	8		
4	D	257	Total	C	N	O	S	0	0
			2066	1306	377	375	8		
4	E	257	Total	C	N	O	S	0	0
			2066	1306	377	375	8		
4	F	257	Total	C	N	O	S	0	0
			2066	1306	377	375	8		
4	G	257	Total	C	N	O	S	0	0
			2066	1306	377	375	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	257	Total	C	N	O	S	0	0
			2066	1306	377	375	8		
4	I	257	Total	C	N	O	S	0	0
			2066	1306	377	375	8		
4	J	257	Total	C	N	O	S	0	0
			2066	1306	377	375	8		
4	K	257	Total	C	N	O	S	0	0
			2066	1306	377	375	8		
4	L	257	Total	C	N	O	S	0	0
			2066	1306	377	375	8		

- Molecule 5 is a protein called Cas12k.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	O	601	Total	C	N	O	S	0	0
			4865	3069	881	900	15		

- Molecule 6 is a protein called TniQ.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Q	164	Total	C	N	O	S	0	0
			1306	832	240	220	14		

- Molecule 7 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	S	87	Total	C	N	O	S	0	0
			702	433	140	128	1		

- Molecule 8 is a protein called TnsB.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	w	14	Total	C	N	O		0	0
			129	83	19	27			
8	x	14	Total	C	N	O		0	0
			129	83	19	27			
8	y	14	Total	C	N	O		0	0
			129	83	19	27			
8	z	14	Total	C	N	O		0	0
			129	83	19	27			
8	W	514	Total	C	N	O	S	0	0
			4122	2570	760	780	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	X	507	Total	C	N	O	S	0	0
			4068	2537	748	771	12		
8	Y	304	Total	C	N	O	S	0	0
			2453	1537	449	457	10		
8	Z	301	Total	C	N	O	S	0	0
			2426	1522	442	452	10		

- Molecule 9 is a DNA chain called LE_R.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	2	29	Total	C	N	O	P	0	0
			593	285	105	175	28		

- Molecule 10 is a DNA chain called RE_F.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	4	46	Total	C	N	O	P	0	0
			941	449	175	271	46		

- Molecule 11 is a DNA chain called RE_R1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	5	28	Total	C	N	O	P	0	0
			573	277	98	171	27		

- Molecule 12 is a DNA chain called RE_R2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	6	13	Total	C	N	O	P	0	0
			263	125	46	79	13		

- Molecule 13 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

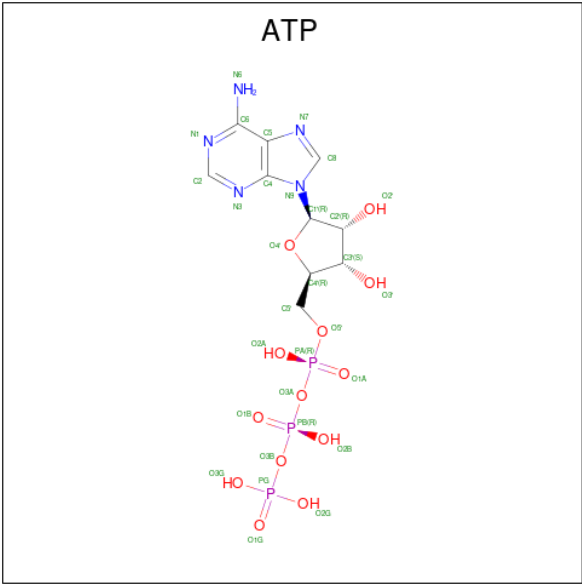
Mol	Chain	Residues	Atoms		AltConf
13	A	1	Total	Mg	0
			1	1	
13	B	1	Total	Mg	0
			1	1	
13	C	1	Total	Mg	0
			1	1	
13	D	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
13	E	1	Total	Mg	0
			1	1	
13	F	1	Total	Mg	0
			1	1	
13	G	1	Total	Mg	0
			1	1	
13	H	1	Total	Mg	0
			1	1	
13	I	1	Total	Mg	0
			1	1	
13	J	1	Total	Mg	0
			1	1	
13	K	1	Total	Mg	0
			1	1	
13	L	1	Total	Mg	0
			1	1	
13	W	1	Total	Mg	0
			1	1	
13	X	1	Total	Mg	0
			1	1	

- Molecule 14 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

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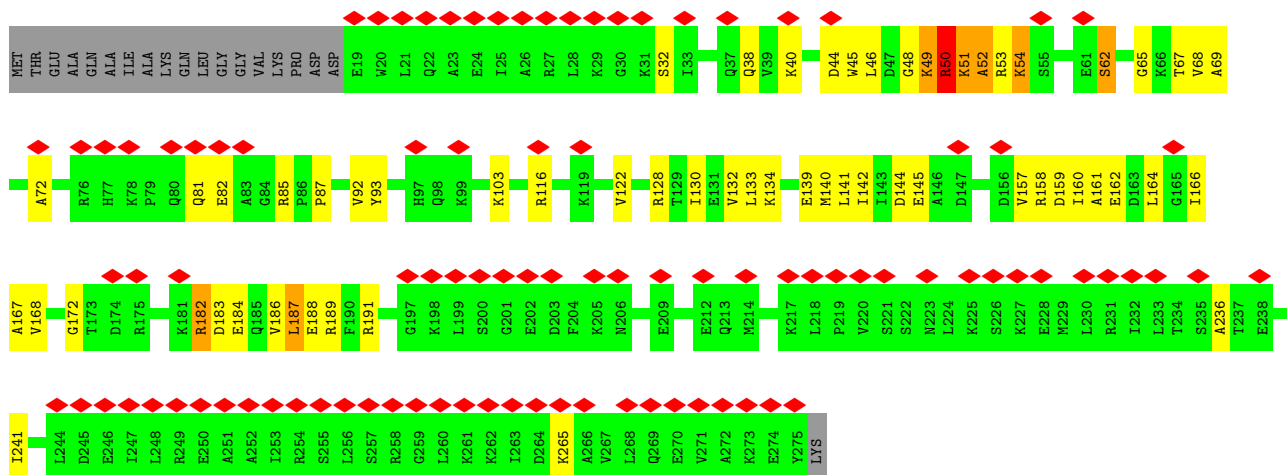
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Mol	Chain	Residues	Atoms					AltConf
14	B	1	Total 31	C 10	N 5	O 13	P 3	0
14	C	1	Total 31	C 10	N 5	O 13	P 3	0
14	D	1	Total 31	C 10	N 5	O 13	P 3	0
14	E	1	Total 31	C 10	N 5	O 13	P 3	0
14	F	1	Total 31	C 10	N 5	O 13	P 3	0
14	G	1	Total 31	C 10	N 5	O 13	P 3	0
14	H	1	Total 31	C 10	N 5	O 13	P 3	0
14	I	1	Total 31	C 10	N 5	O 13	P 3	0
14	J	1	Total 31	C 10	N 5	O 13	P 3	0
14	K	1	Total 31	C 10	N 5	O 13	P 3	0
14	L	1	Total 31	C 10	N 5	O 13	P 3	0

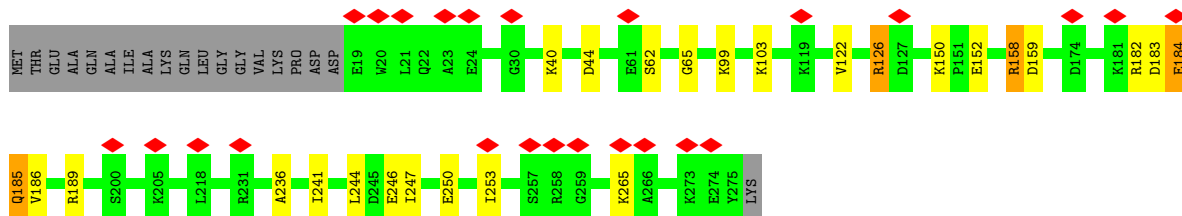
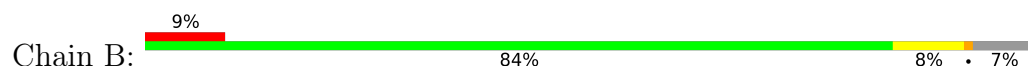




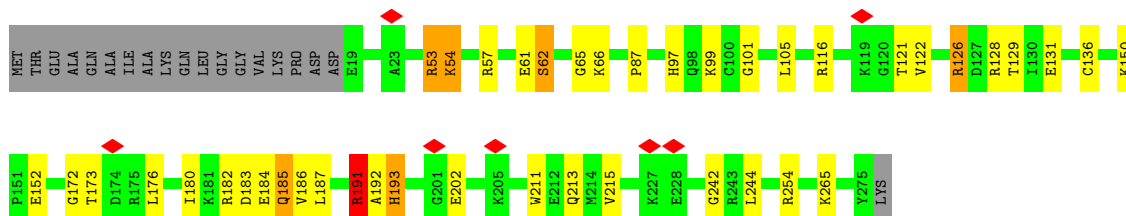
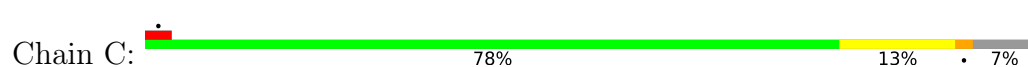
• Molecule 4: TnsC



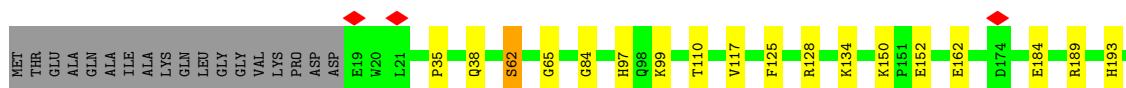
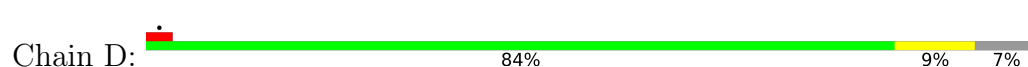
• Molecule 4: TnsC

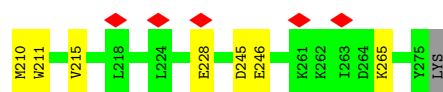


• Molecule 4: TnsC

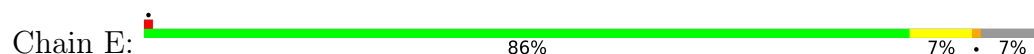


• Molecule 4: TnsC

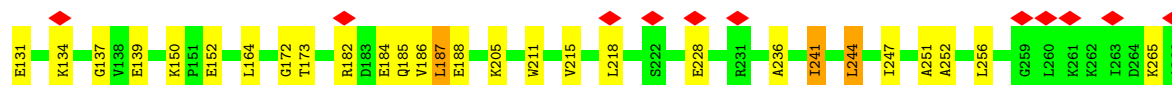
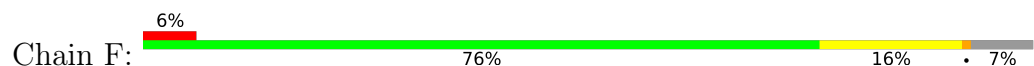




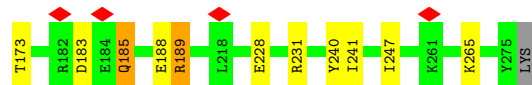
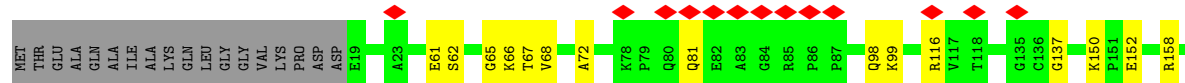
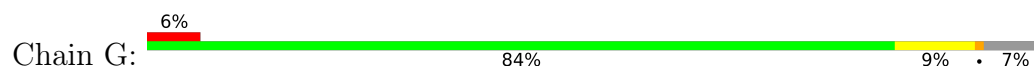
- Molecule 4: TnsC



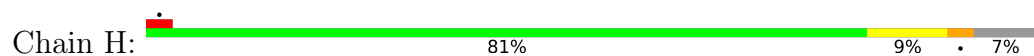
- Molecule 4: TnsC



- Molecule 4: TnsC

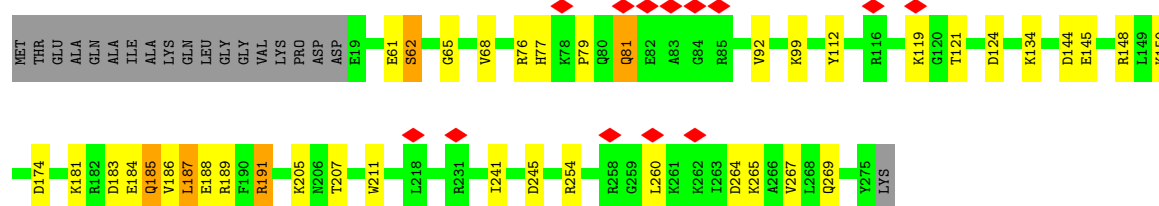


- Molecule 4: TnsC



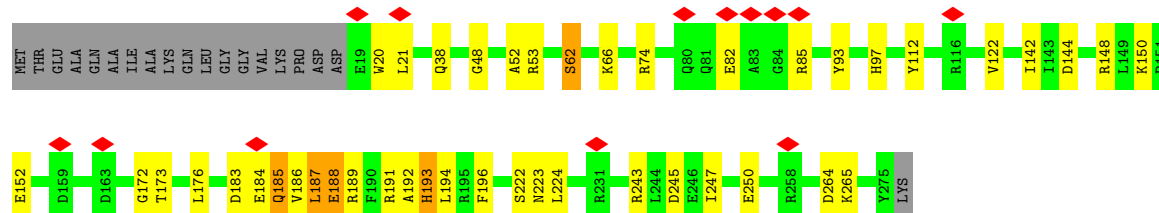
- Molecule 4: TnsC

Chain I: 



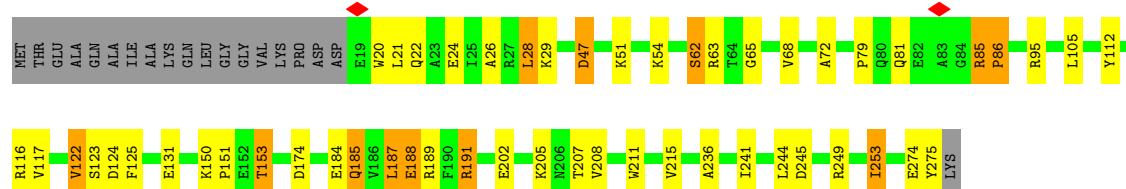
- Molecule 4: TnsC

Chain J: 



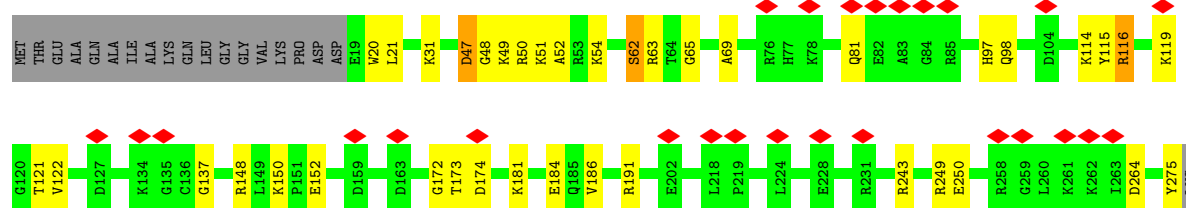
- Molecule 4: TnsC

Chain K: 



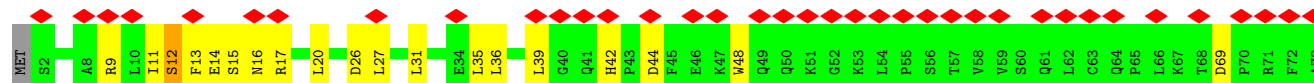
- Molecule 4: TnsC

Chain L: 



- Molecule 5: Cas12k

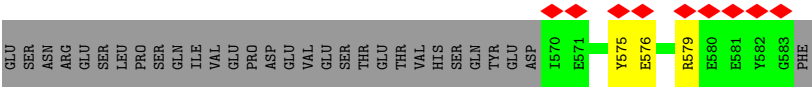
Chain O: 



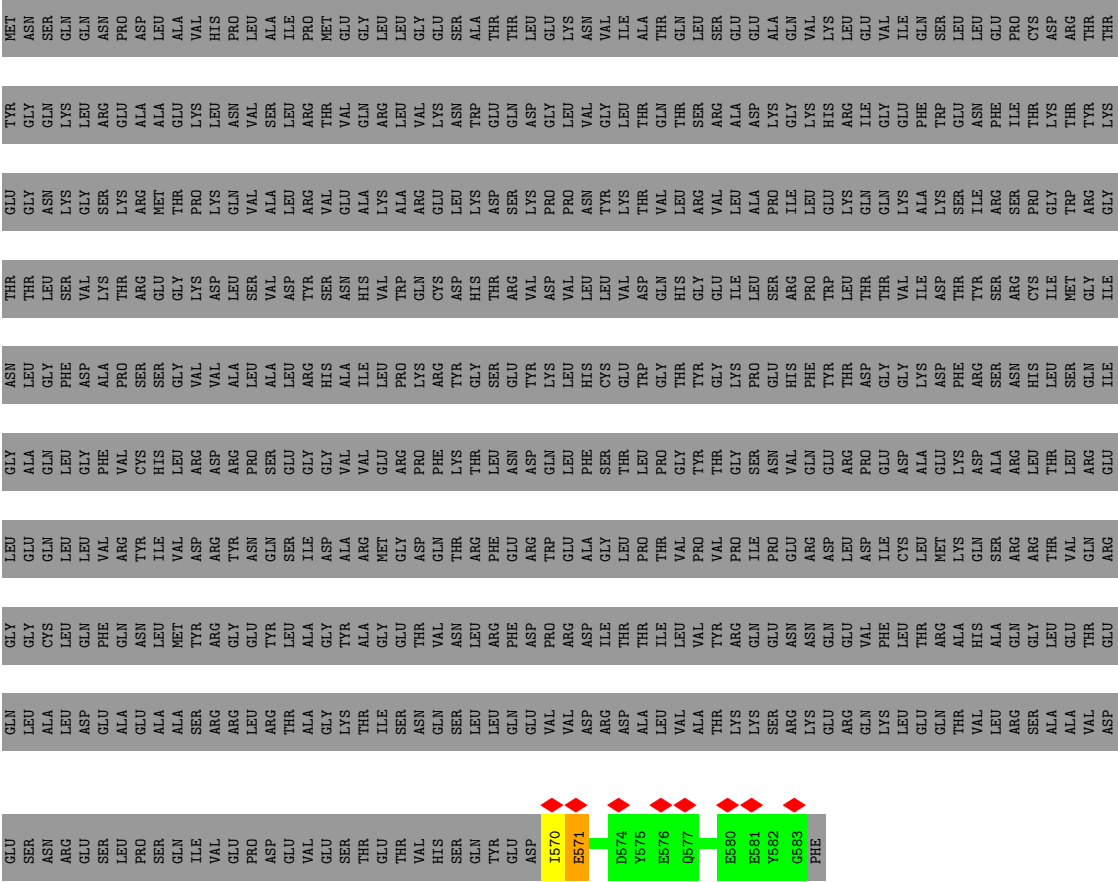
- Molecule 8: TnsB



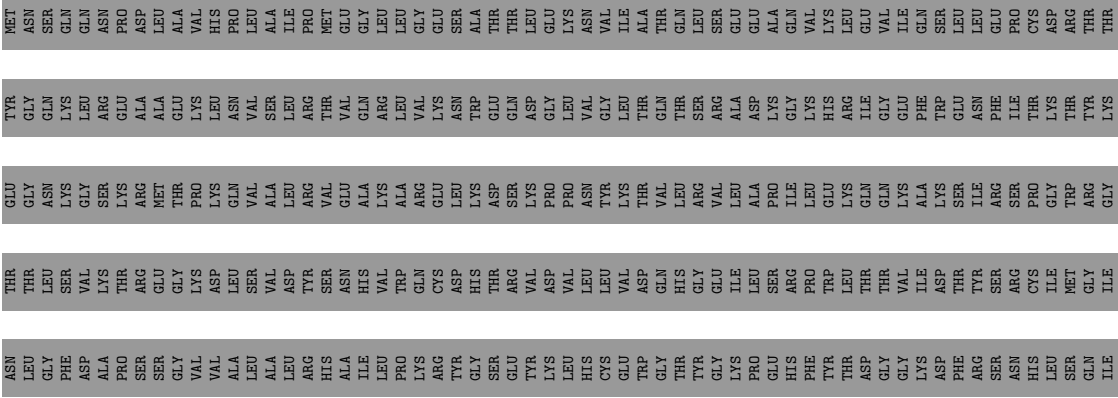
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LEU	GLN	CYS	GLN	ALA	GLN	ALA	GLN	GLY	GLY	THR	THR	GLN	ASN	THR	THR	GLY	ASN	GLN	ASN
ALA	LEU	LEU	LEU	LEU	LEU	LEU	LEU	PHE	PHE	VAL	VAL	GLY	GLY	VAL	VAL	GLY	GLY	GLN	GLN
GLY	GLY	PHE	GLN	VAL	VAL	VAL	PHE	VAL	ALA	THR	THR	GLY	GLY	THR	THR	GLY	GLY	ASN	ASN
ALA	GLN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



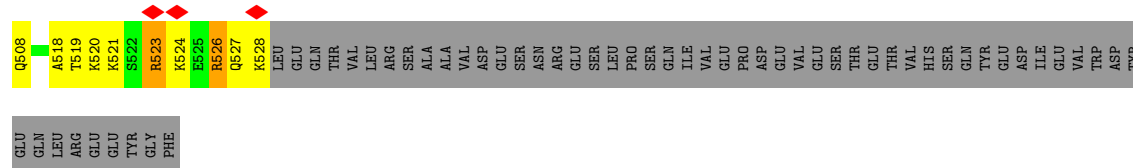
• Molecule 8: TnsB

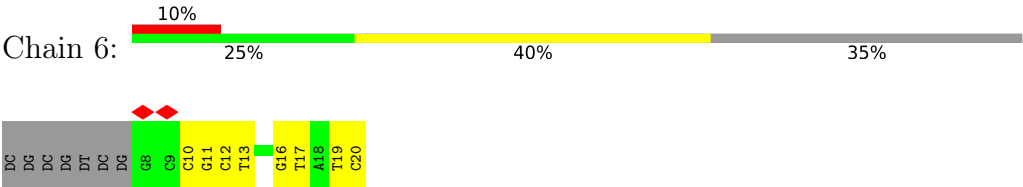


• Molecule 8: TnsB









4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	188055	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	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	2.956	Depositor
Minimum map value	-1.515	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.063	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	576.18, 576.18, 576.18	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.067, 1.067, 1.067	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, 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	1	0.24	0/2280	0.49	2/3516 (0.1%)
2	3	0.33	0/1143	0.70	3/1759 (0.2%)
3	7	0.16	0/5470	0.33	7/8517 (0.1%)
4	A	1.16	11/2097 (0.5%)	1.29	14/2817 (0.5%)
4	B	1.08	10/2097 (0.5%)	1.30	8/2817 (0.3%)
4	C	1.16	10/2097 (0.5%)	1.32	8/2817 (0.3%)
4	D	0.92	0/2097	1.30	5/2817 (0.2%)
4	E	1.01	5/2097 (0.2%)	1.25	2/2817 (0.1%)
4	F	1.15	11/2097 (0.5%)	1.31	12/2817 (0.4%)
4	G	0.97	2/2097 (0.1%)	1.33	7/2817 (0.2%)
4	H	1.10	10/2097 (0.5%)	1.29	4/2817 (0.1%)
4	I	1.00	6/2097 (0.3%)	1.27	8/2817 (0.3%)
4	J	1.11	8/2097 (0.4%)	1.37	8/2817 (0.3%)
4	K	1.15	11/2097 (0.5%)	1.41	21/2817 (0.7%)
4	L	1.08	7/2097 (0.3%)	1.33	13/2817 (0.5%)
5	O	0.77	1/4952 (0.0%)	1.20	6/6677 (0.1%)
6	Q	0.81	1/1345 (0.1%)	1.28	4/1819 (0.2%)
7	S	0.90	0/710	1.33	1/950 (0.1%)
8	W	0.86	0/4192	1.18	1/5659 (0.0%)
8	X	0.87	3/4137 (0.1%)	1.31	17/5585 (0.3%)
8	Y	0.85	1/2499 (0.0%)	1.25	11/3379 (0.3%)
8	Z	0.81	2/2472 (0.1%)	1.30	18/3345 (0.5%)
8	w	0.76	0/132	1.22	0/178
8	x	1.00	0/132	1.15	0/178
8	y	0.85	0/132	1.36	2/178 (1.1%)
8	z	0.78	0/132	1.26	0/178
9	2	0.17	0/664	0.35	0/1024
10	4	0.17	0/1056	0.34	0/1626
11	5	0.17	0/641	0.37	0/989
12	6	0.16	0/293	0.30	0/449
All	All	0.87	99/57546 (0.2%)	1.15	182/79810 (0.2%)

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
4	C	0	1
4	D	0	1
4	F	0	1
4	G	0	2
4	H	0	1
4	K	0	1
4	L	0	1
8	W	0	3
8	X	0	3
8	Y	0	3
8	Z	0	1
8	x	0	1
All	All	0	19

All (99) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	Z	463	ASN	C-N	-8.02	1.22	1.33
4	B	186	VAL	C-O	-7.50	1.15	1.24
8	X	355	ARG	C-N	-7.43	1.23	1.33
4	A	38	GLN	C-O	-7.23	1.15	1.24
4	B	184	GLU	C-O	-7.15	1.15	1.24
4	J	247	ILE	C-O	-7.13	1.16	1.24
4	C	184	GLU	C-O	-7.11	1.15	1.24
4	H	184	GLU	C-O	-7.08	1.15	1.24
4	C	105	LEU	C-O	-7.07	1.15	1.24
4	F	38	GLN	C-O	-7.04	1.15	1.24
4	E	184	GLU	C-O	-7.00	1.15	1.24
4	A	184	GLU	C-O	-7.00	1.15	1.24
4	F	105	LEU	C-O	-6.94	1.16	1.24
4	F	186	VAL	C-O	-6.89	1.15	1.24
4	L	186	VAL	C-O	-6.86	1.16	1.24
4	A	186	VAL	C-O	-6.80	1.15	1.24
8	Z	462	GLU	C-N	-6.80	1.23	1.33
4	E	186	VAL	C-O	-6.79	1.15	1.24
4	A	49	LYS	C-N	6.78	1.43	1.33
4	C	186	VAL	C-O	-6.77	1.15	1.24
4	K	244	LEU	C-O	-6.76	1.16	1.24
4	B	244	LEU	C-O	-6.73	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	184	GLU	C-O	-6.69	1.15	1.24
4	F	122	VAL	C-O	-6.65	1.16	1.24
4	J	184	GLU	C-O	-6.64	1.15	1.24
4	J	186	VAL	C-O	-6.64	1.15	1.24
4	L	50	ARG	C-O	-6.63	1.16	1.24
4	B	247	ILE	C-O	-6.63	1.16	1.24
4	I	184	GLU	C-O	-6.62	1.15	1.24
4	I	186	VAL	C-O	-6.62	1.16	1.24
4	H	244	LEU	C-O	-6.60	1.16	1.24
4	F	244	LEU	C-O	-6.55	1.16	1.24
4	H	186	VAL	C-O	-6.55	1.16	1.24
4	G	247	ILE	C-O	-6.53	1.16	1.24
4	F	247	ILE	C-O	-6.49	1.16	1.24
4	C	122	VAL	C-O	-6.46	1.16	1.24
4	C	129	THR	C-O	-6.24	1.17	1.24
4	F	129	THR	C-O	-6.24	1.17	1.24
4	A	38	GLN	CA-C	-6.16	1.44	1.52
4	F	38	GLN	CA-C	-6.07	1.45	1.52
4	J	245	ASP	C-O	-6.07	1.17	1.24
4	K	245	ASP	C-O	-6.07	1.17	1.24
4	I	187	LEU	C-O	-6.04	1.17	1.24
4	K	187	LEU	C-O	-6.02	1.17	1.24
4	K	241	ILE	C-O	-6.01	1.16	1.24
4	C	185	GLN	C-O	-5.99	1.17	1.24
4	H	241	ILE	C-O	-5.99	1.16	1.24
4	K	28	LEU	CA-C	-5.94	1.45	1.52
4	I	185	GLN	C-O	-5.93	1.17	1.24
4	F	187	LEU	C-O	-5.92	1.17	1.24
4	H	185	GLN	C-O	-5.92	1.17	1.24
8	X	131	PRO	C-O	-5.89	1.16	1.24
4	J	187	LEU	C-O	-5.82	1.17	1.24
4	L	54	LYS	C-O	-5.81	1.16	1.23
4	B	241	ILE	C-O	-5.80	1.16	1.24
4	A	187	LEU	C-O	-5.80	1.17	1.24
4	K	185	GLN	C-O	-5.76	1.17	1.24
4	A	241	ILE	C-O	-5.76	1.16	1.24
4	A	54	LYS	C-O	-5.75	1.16	1.24
4	F	241	ILE	C-O	-5.74	1.16	1.24
5	O	12	SER	CA-CB	-5.74	1.44	1.53
4	E	185	GLN	C-O	-5.70	1.17	1.24
4	C	126	ARG	C-O	-5.69	1.17	1.24
4	A	183	ASP	C-O	-5.69	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	185	GLN	C-O	-5.69	1.17	1.24
4	C	191	ARG	CA-C	-5.68	1.47	1.53
4	C	183	ASP	C-O	-5.67	1.17	1.23
4	J	183	ASP	C-O	-5.66	1.17	1.23
4	H	187	LEU	C-O	-5.66	1.17	1.24
4	E	187	LEU	C-O	-5.63	1.17	1.24
4	E	183	ASP	C-O	-5.62	1.17	1.24
4	L	49	LYS	N-CA	-5.62	1.39	1.46
4	I	183	ASP	C-O	-5.60	1.17	1.24
4	L	47	ASP	C-O	-5.53	1.17	1.24
4	K	47	ASP	C-O	-5.53	1.17	1.24
4	H	47	ASP	C-O	-5.51	1.17	1.24
4	B	183	ASP	C-O	-5.49	1.17	1.23
4	G	183	ASP	C-O	-5.43	1.17	1.23
4	K	24	GLU	C-O	-5.41	1.17	1.24
4	B	253	ILE	C-O	-5.39	1.18	1.24
4	H	183	ASP	C-O	-5.39	1.17	1.23
8	Y	251	VAL	C-N	-5.35	1.27	1.33
4	H	46	LEU	C-O	-5.33	1.17	1.24
4	A	46	LEU	C-O	-5.33	1.17	1.24
4	L	50	ARG	CA-C	-5.29	1.45	1.52
4	B	246	GLU	CA-C	-5.27	1.46	1.52
4	B	126	ARG	C-O	-5.25	1.17	1.24
8	X	262	PRO	C-O	-5.25	1.17	1.23
4	K	253	ILE	C-O	-5.22	1.18	1.24
4	C	176	LEU	C-O	-5.15	1.18	1.24
4	L	49	LYS	CA-C	-5.09	1.45	1.52
4	I	188	GLU	C-O	-5.08	1.17	1.24
4	J	176	LEU	C-O	-5.06	1.18	1.24
4	K	211	TRP	CA-C	-5.05	1.46	1.52
6	Q	157	PRO	C-O	-5.05	1.17	1.23
4	J	188	GLU	C-O	-5.04	1.17	1.24
4	F	251	ALA	C-O	-5.02	1.18	1.24
4	A	188	GLU	C-O	-5.01	1.17	1.24
4	H	188	GLU	C-O	-5.00	1.17	1.24

All (182) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	34	DC	P-O3'-C3'	-9.67	105.69	120.20
8	Y	223	ARG	CA-C-N	9.42	130.12	120.14
8	Y	223	ARG	C-N-CA	9.42	130.12	120.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Q	94	HIS	CB-CA-C	-9.17	95.22	110.72
8	Z	504	GLN	CB-CA-C	-8.26	107.05	116.63
4	K	215	VAL	N-CA-C	8.25	118.65	111.56
4	K	85	ARG	CA-C-N	8.23	128.86	120.38
4	K	85	ARG	C-N-CA	8.23	128.86	120.38
4	K	208	VAL	N-CA-C	-8.22	102.53	110.42
4	H	191	ARG	N-CA-C	8.17	120.18	111.28
4	L	191	ARG	N-CA-C	8.11	120.12	111.28
4	G	265	LYS	N-CA-C	8.08	120.81	111.11
4	A	191	ARG	N-CA-C	8.07	120.08	111.28
4	D	265	LYS	N-CA-C	8.04	120.76	111.11
4	J	191	ARG	N-CA-C	8.04	120.04	111.28
4	C	265	LYS	N-CA-C	8.04	120.75	111.11
4	I	191	ARG	N-CA-C	8.03	120.03	111.28
4	K	191	ARG	N-CA-C	8.02	120.02	111.28
4	F	265	LYS	N-CA-C	8.01	120.72	111.11
3	7	230	G	P-O3'-C3'	-8.00	108.21	120.20
8	Z	299	GLN	N-CA-C	-8.00	102.25	110.97
4	L	48	GLY	N-CA-C	-7.97	103.26	112.50
4	F	205	LYS	N-CA-C	7.83	120.51	111.11
8	Y	339	THR	N-CA-C	-7.78	103.79	113.28
1	1	30	DC	P-O3'-C3'	-7.70	108.64	120.20
3	7	48	U	P-O3'-C3'	-7.53	108.90	120.20
4	I	62	SER	N-CA-C	7.53	121.57	112.38
3	7	50	A	P-O3'-C3'	-7.53	108.91	120.20
4	K	62	SER	N-CA-C	7.49	121.51	112.38
4	K	205	LYS	N-CA-C	7.48	120.38	111.33
4	C	62	SER	N-CA-C	7.47	121.50	112.38
4	J	48	GLY	N-CA-C	-7.47	103.45	112.49
4	A	62	SER	N-CA-C	7.46	121.48	112.38
4	L	62	SER	N-CA-C	7.45	121.46	112.38
4	F	62	SER	N-CA-C	7.44	121.46	112.38
4	J	62	SER	N-CA-C	7.42	121.43	112.38
4	B	62	SER	N-CA-C	7.38	121.39	112.38
4	I	205	LYS	N-CA-C	7.34	120.22	111.33
8	Z	332	PHE	N-CA-C	7.32	119.25	111.28
4	D	62	SER	N-CA-C	7.15	121.44	112.87
8	X	157	LEU	N-CA-C	-7.10	103.48	111.07
4	K	86	PRO	CA-C-N	7.04	126.97	120.21
4	K	86	PRO	C-N-CA	7.04	126.97	120.21
4	L	52	ALA	N-CA-C	-7.01	104.70	113.18
4	K	24	GLU	N-CA-C	7.00	120.92	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	193	HIS	N-CA-C	6.97	119.78	108.76
4	L	98	GLN	N-CA-C	6.88	119.94	110.24
8	X	123	ASN	N-CA-C	-6.88	103.47	112.41
4	I	188	GLU	N-CA-C	6.85	119.77	111.82
4	J	188	GLU	N-CA-C	6.84	119.75	111.82
4	A	188	GLU	N-CA-C	6.83	119.75	111.82
4	K	188	GLU	N-CA-C	6.83	119.74	111.82
8	Z	369	ILE	N-CA-C	6.82	116.97	110.42
4	E	188	GLU	N-CA-C	6.82	119.73	111.82
4	F	188	GLU	N-CA-C	6.81	119.72	111.82
8	W	272	HIS	N-CA-C	-6.79	105.62	114.04
4	H	188	GLU	N-CA-C	6.77	119.67	111.82
8	X	110	PHE	N-CA-C	-6.72	103.88	111.07
2	3	37	DT	P-O3'-C3'	-6.68	110.18	120.20
8	X	39	SER	N-CA-C	6.66	119.36	111.71
8	Y	332	PHE	N-CA-C	6.60	119.31	111.33
4	J	52	ALA	N-CA-C	-6.56	104.75	112.89
3	7	228	A	P-O3'-C3'	-6.55	110.38	120.20
8	Z	230	ILE	N-CA-C	6.41	118.01	108.46
8	Z	504	GLN	N-CA-C	6.41	118.91	108.08
8	X	329	ASP	N-CA-C	6.39	119.23	111.82
4	L	50	ARG	N-CA-C	6.29	118.13	111.28
8	X	167	GLN	N-CA-C	-6.28	104.51	111.36
8	X	315	SER	N-CA-C	-6.28	105.28	114.39
4	H	172	GLY	N-CA-C	6.23	119.58	110.80
8	Z	335	LEU	CA-C-N	6.19	126.56	119.93
8	Z	335	LEU	C-N-CA	6.19	126.56	119.93
8	Y	335	LEU	CA-C-N	6.19	126.56	119.93
8	Y	335	LEU	C-N-CA	6.19	126.56	119.93
8	Z	523	ARG	N-CA-C	-6.15	104.58	111.28
4	J	172	GLY	N-CA-C	6.13	119.45	110.80
4	F	172	GLY	N-CA-C	6.10	119.51	110.42
4	L	172	GLY	N-CA-C	6.09	119.39	110.80
4	C	172	GLY	N-CA-C	6.08	119.49	110.42
4	E	172	GLY	N-CA-C	6.06	119.45	110.42
4	C	105	LEU	N-CA-C	6.05	117.88	111.28
4	A	172	GLY	N-CA-C	6.05	119.43	110.42
4	B	158	ARG	CA-C-N	6.04	128.29	120.44
4	B	158	ARG	C-N-CA	6.04	128.29	120.44
4	H	62	SER	N-CA-C	6.01	119.08	111.69
7	S	13	SER	N-CA-C	-6.00	105.97	113.28
2	3	26	DA	P-O3'-C3'	-5.96	111.27	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	207	THR	O-C-N	5.93	128.41	122.12
8	Z	258	HIS	N-CA-C	-5.90	104.54	110.97
4	L	69	ALA	CA-C-N	5.89	128.45	120.44
4	L	69	ALA	C-N-CA	5.89	128.45	120.44
4	F	105	LEU	N-CA-C	5.88	117.69	111.28
3	7	229	A	P-O3'-C3'	-5.88	111.39	120.20
3	7	227	A	P-O3'-C3'	-5.87	111.40	120.20
8	X	426	PHE	CA-C-N	-5.87	114.03	122.36
8	X	426	PHE	C-N-CA	-5.87	114.03	122.36
8	Z	445	ASN	CA-CB-CG	5.86	118.46	112.60
4	D	193	HIS	N-CA-C	5.85	118.18	108.99
4	A	52	ALA	N-CA-C	-5.84	106.06	112.72
8	X	165	GLU	N-CA-C	-5.82	105.02	111.36
4	B	159	ASP	CA-C-N	5.80	128.08	120.60
4	B	159	ASP	C-N-CA	5.80	128.08	120.60
3	7	47	G	P-O3'-C3'	-5.77	111.55	120.20
8	Z	355	ARG	N-CA-C	5.76	118.61	109.50
8	X	40	GLU	N-CA-C	5.76	117.25	110.97
4	B	265	LYS	N-CA-C	5.75	120.85	111.37
4	A	265	LYS	N-CA-C	5.74	120.85	111.37
6	Q	163	LYS	N-CA-C	-5.71	106.14	113.23
4	F	101	GLY	CA-C-N	5.67	125.52	119.28
4	F	101	GLY	C-N-CA	5.67	125.52	119.28
8	Z	521	LYS	N-CA-C	-5.66	105.11	111.28
8	X	132	LYS	N-CA-C	-5.64	105.21	111.36
4	G	68	VAL	N-CA-C	5.58	116.32	110.62
4	I	79	PRO	N-CA-C	5.57	119.96	111.15
4	A	68	VAL	N-CA-C	5.54	116.27	110.62
4	C	101	GLY	CA-C-N	5.54	125.37	119.28
4	C	101	GLY	C-N-CA	5.54	125.37	119.28
5	O	69	ASP	CA-C-N	5.54	125.89	119.47
5	O	69	ASP	C-N-CA	5.54	125.89	119.47
8	Z	265	TYR	N-CA-C	5.52	118.28	110.50
1	1	32	DA	P-O3'-C3'	-5.52	111.92	120.20
5	O	131	ALA	N-CA-C	-5.50	105.29	111.28
6	Q	160	GLU	N-CA-C	-5.50	106.62	113.38
4	K	68	VAL	N-CA-C	5.44	116.17	110.62
8	Z	339	THR	N-CA-C	-5.44	103.80	110.65
4	G	137	GLY	N-CA-C	-5.43	103.43	111.03
4	L	98	GLN	N-CA-CB	-5.42	101.08	109.69
4	L	264	ASP	CA-CB-CG	5.41	118.01	112.60
8	X	355	ARG	O-C-N	-5.41	115.87	122.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	X	150	PRO	N-CA-C	-5.40	104.12	110.70
4	A	69	ALA	CA-C-N	5.35	127.89	120.29
4	A	69	ALA	C-N-CA	5.35	127.89	120.29
4	G	72	ALA	N-CA-C	-5.34	105.46	111.28
4	K	81	GLN	N-CA-C	5.33	118.12	108.69
4	F	137	GLY	N-CA-C	-5.32	103.58	111.03
4	J	250	GLU	N-CA-C	-5.30	105.58	111.36
4	C	193	HIS	CA-C-N	-5.30	114.25	122.09
4	C	193	HIS	C-N-CA	-5.30	114.25	122.09
4	K	72	ALA	N-CA-C	-5.30	105.50	111.28
4	L	81	GLN	N-CA-C	5.30	118.06	108.69
4	A	72	ALA	N-CA-C	-5.29	105.51	111.28
8	Z	232	THR	N-CA-C	5.29	119.36	113.01
8	Y	265	TYR	N-CA-C	5.29	118.31	110.48
8	Y	232	THR	N-CA-C	5.28	119.35	113.01
8	y	571	GLU	CA-C-N	5.28	130.27	122.94
8	y	571	GLU	C-N-CA	5.28	130.27	122.94
8	X	291	ASP	N-CA-C	-5.28	105.61	111.36
4	L	137	GLY	N-CA-C	-5.27	103.65	111.03
8	X	526	ARG	NE-CZ-NH2	5.27	123.94	119.20
4	B	250	GLU	N-CA-C	-5.26	105.62	111.36
4	G	81	GLN	N-CA-C	5.26	118.00	108.69
8	X	295	ASN	N-CA-C	-5.24	105.65	111.36
4	K	122	VAL	N-CA-C	-5.24	105.43	110.72
6	Q	121	LYS	CA-C-O	-5.23	114.99	121.06
5	O	26	ASP	CA-C-N	5.23	127.71	120.29
5	O	26	ASP	C-N-CA	5.23	127.71	120.29
4	A	52	ALA	CA-C-N	-5.22	115.10	122.46
4	A	52	ALA	C-N-CA	-5.22	115.10	122.46
4	F	114	LYS	N-CA-C	5.19	118.75	111.74
4	K	22	GLN	N-CA-C	5.19	118.07	111.69
4	F	38	GLN	N-CA-C	-5.19	105.71	111.36
4	K	174	ASP	CA-C-N	5.18	127.75	120.28
4	K	174	ASP	C-N-CA	5.18	127.75	120.28
4	D	134	LYS	CA-C-N	5.18	125.58	119.94
4	D	134	LYS	C-N-CA	5.18	125.58	119.94
4	A	38	GLN	N-CA-C	-5.16	105.73	111.36
4	K	26	ALA	N-CA-C	5.15	116.89	111.28
8	Y	484	LEU	N-CA-C	5.10	116.83	111.28
5	O	414	THR	N-CA-C	-5.08	106.92	113.01
4	I	81	GLN	N-CA-C	5.07	116.95	108.99
8	Y	240	ILE	N-CA-C	5.07	117.32	108.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	241	ILE	CA-C-N	5.06	125.55	119.94
4	G	241	ILE	C-N-CA	5.06	125.55	119.94
4	F	236	ALA	N-CA-C	5.04	116.78	111.28
4	K	236	ALA	N-CA-C	5.04	116.78	111.28
4	B	236	ALA	N-CA-C	5.02	116.75	111.28
8	Z	269	TYR	N-CA-C	-5.01	107.17	113.28
8	Z	371	ASP	N-CA-C	5.01	119.54	113.38
4	A	236	ALA	N-CA-C	5.00	116.74	111.28
4	I	134	LYS	CA-C-N	5.00	125.51	120.00
4	I	134	LYS	C-N-CA	5.00	125.51	120.00
8	Y	269	TYR	N-CA-C	-5.00	107.18	113.28

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	C	254	ARG	Sidechain
4	D	128	ARG	Sidechain
4	F	182	ARG	Sidechain
4	G	189	ARG	Sidechain
4	G	240	TYR	Sidechain
4	H	27	ARG	Sidechain
4	K	95	ARG	Sidechain
4	L	116	ARG	Sidechain
8	W	166	LYS	Mainchain
8	W	367	ARG	Sidechain
8	W	372	ARG	Sidechain
8	X	223	ARG	Sidechain
8	X	367	ARG	Sidechain
8	X	416	ARG	Sidechain
8	Y	448	PHE	Mainchain
8	Y	523	ARG	Sidechain
8	Y	526	ARG	Sidechain
8	Z	523	ARG	Sidechain
8	x	575	TYR	Sidechain

5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	2031	0	1118	147	0
2	3	1022	0	569	59	0
3	7	4896	0	2471	100	0
4	A	2066	0	2155	66	0
4	B	2066	0	2154	33	0
4	C	2066	0	2157	68	0
4	D	2066	0	2157	39	0
4	E	2066	0	2157	26	0
4	F	2066	0	2158	62	0
4	G	2066	0	2158	27	0
4	H	2066	0	2157	45	0
4	I	2066	0	2157	82	0
4	J	2066	0	2156	72	0
4	K	2066	0	2154	81	0
4	L	2066	0	2155	61	0
5	O	4865	0	4926	195	0
6	Q	1306	0	1290	48	0
7	S	702	0	721	18	0
8	W	4122	0	4147	114	0
8	X	4068	0	4078	121	0
8	Y	2453	0	2421	45	0
8	Z	2426	0	2389	19	0
8	w	129	0	110	0	0
8	x	129	0	110	14	0
8	y	129	0	110	5	0
8	z	129	0	110	0	0
9	2	593	0	331	43	0
10	4	941	0	518	60	0
11	5	573	0	322	38	0
12	6	263	0	146	27	0
13	A	1	0	0	1	0
13	B	1	0	0	0	0
13	C	1	0	0	0	0
13	D	1	0	0	0	0
13	E	1	0	0	0	0
13	F	1	0	0	2	0
13	G	1	0	0	2	0
13	H	1	0	0	0	0
13	I	1	0	0	0	0
13	J	1	0	0	0	0
13	K	1	0	0	0	0
13	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	W	1	0	0	0	0
13	X	1	0	0	0	0
14	A	31	0	12	3	0
14	B	31	0	12	8	0
14	C	31	0	12	4	0
14	D	31	0	12	5	0
14	E	31	0	12	2	0
14	F	31	0	12	3	0
14	G	31	0	12	2	0
14	H	31	0	12	3	0
14	I	31	0	12	3	0
14	J	31	0	12	2	0
14	K	31	0	12	1	0
14	L	31	0	12	7	0
All	All	55955	0	51906	1223	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 11.

All (1223) 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)
5:O:412:SER:CB	5:O:415:GLN:CD	1.75	1.59
3:7:86:G:H1	5:O:300:ARG:NH2	1.09	1.51
4:F:218:LEU:CD2	4:F:256:LEU:HD11	1.43	1.49
4:I:191:ARG:CZ	4:J:243:ARG:NH2	1.73	1.47
1:1:-24:DC:C6	8:W:77:ARG:NH2	1.88	1.41
5:O:292:VAL:HB	5:O:304:HIS:CE1	1.55	1.38
4:J:53:ARG:CG	4:K:29:LYS:NZ	1.87	1.37
4:G:158:ARG:CD	4:G:189:ARG:NH1	1.86	1.36
4:G:158:ARG:CD	4:G:189:ARG:HH11	1.34	1.36
5:O:39:LEU:HD23	5:O:91:TYR:OH	1.23	1.35
8:X:58:ARG:NH2	10:4:-27:DC:O2	1.60	1.35
5:O:42:HIS:CE1	5:O:44:ASP:HB2	1.61	1.34
8:x:576:GLU:HG3	8:x:579:ARG:NH2	1.39	1.33
4:I:211:TRP:CZ2	4:I:241:ILE:HD11	1.63	1.32
4:I:191:ARG:NE	4:J:243:ARG:HH21	1.30	1.28
1:1:36:DG:C3'	4:I:119:LYS:HE2	1.63	1.27
4:C:211:TRP:CZ3	4:C:215:VAL:HG21	1.69	1.27
4:F:218:LEU:HD21	4:F:256:LEU:CD1	1.64	1.26
5:O:412:SER:CB	5:O:415:GLN:NE2	1.98	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:158:ARG:HD2	4:G:189:ARG:NH1	0.95	1.26
5:O:478:LYS:HG2	5:O:485:TYR:CE2	1.70	1.26
5:O:39:LEU:CD2	5:O:91:TYR:OH	1.83	1.25
2:3:-1:DT:OP1	5:O:414:THR:HB	1.35	1.25
1:1:42:DC:C5'	4:L:119:LYS:HD2	1.69	1.22
1:1:-24:DC:C5	8:W:77:ARG:NH1	2.07	1.22
1:1:60:DC:H2''	5:O:351:ASN:OD1	1.05	1.21
4:F:131:GLU:OE1	4:L:181:LYS:NZ	1.73	1.21
4:J:53:ARG:HG3	4:K:29:LYS:CE	1.71	1.21
4:I:191:ARG:NH2	4:J:243:ARG:NH2	1.87	1.20
2:3:-5:DT:P	5:O:309:SER:HG	1.65	1.19
4:J:53:ARG:HG3	4:K:29:LYS:NZ	1.51	1.19
5:O:292:VAL:CB	5:O:304:HIS:CE1	2.26	1.18
1:1:36:DG:H5'	4:I:119:LYS:HZ1	1.08	1.18
3:7:241:U:OP1	5:O:579:LYS:NZ	1.76	1.17
1:1:-24:DC:C5	8:W:77:ARG:CZ	2.26	1.17
2:3:17:DG:C6	5:O:567:PHE:HE2	1.61	1.17
4:J:53:ARG:CG	4:K:29:LYS:CE	2.21	1.17
1:1:60:DC:C2'	5:O:351:ASN:OD1	1.94	1.16
4:I:191:ARG:NE	4:J:243:ARG:NH2	1.89	1.15
4:K:20:TRP:CZ3	4:K:21:LEU:HD23	1.80	1.15
1:1:63:DC:OP1	5:O:343:SER:OG	1.64	1.15
2:3:17:DG:C5	5:O:567:PHE:HE2	1.65	1.14
5:O:13:PHE:CE1	5:O:15:SER:HB2	1.82	1.14
1:1:42:DC:O4'	4:L:119:LYS:NZ	1.79	1.13
1:1:36:DG:H3'	4:I:119:LYS:CE	1.79	1.12
8:x:576:GLU:CG	8:x:579:ARG:NH2	2.11	1.12
8:X:380:ARG:HH12	9:2:3:DT:H3'	1.03	1.12
4:H:185:GLN:HE22	4:I:62:SER:CB	1.62	1.12
4:H:185:GLN:HE22	4:I:62:SER:HB2	0.97	1.12
5:O:17:ARG:HH12	5:O:371:LEU:HB2	1.02	1.11
2:3:-1:DT:O3'	5:O:418:LEU:HD13	1.51	1.11
5:O:81:MET:O	5:O:85:HIS:ND1	1.84	1.10
4:J:53:ARG:CG	4:K:29:LYS:HZ2	1.57	1.10
5:O:17:ARG:HH22	5:O:371:LEU:N	1.50	1.09
5:O:42:HIS:HE1	5:O:44:ASP:CB	1.64	1.09
4:A:141:LEU:HD11	4:A:168:VAL:HG13	1.11	1.09
5:O:17:ARG:NH2	5:O:371:LEU:H	1.50	1.09
3:7:86:G:N1	5:O:300:ARG:NH2	1.75	1.09
4:F:218:LEU:HD22	4:F:256:LEU:CD2	1.80	1.08
5:O:13:PHE:HE1	5:O:15:SER:HB2	1.08	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:53:ARG:HG2	4:K:29:LYS:HZ2	0.92	1.08
4:J:53:ARG:CG	4:K:29:LYS:HE3	1.83	1.08
8:Y:523:ARG:HG3	8:Y:526:ARG:HE	1.13	1.08
4:H:185:GLN:OE1	4:I:62:SER:HB3	1.52	1.07
8:X:425:GLN:CB	12:6:12:DC:OP1	2.02	1.07
4:A:141:LEU:CD1	4:A:168:VAL:HG13	1.83	1.07
4:I:185:GLN:OE1	4:J:173:THR:HG21	1.55	1.07
1:1:-24:DC:C5	8:W:77:ARG:NH2	2.20	1.06
4:I:211:TRP:HZ2	4:I:241:ILE:CD1	1.68	1.06
1:1:-12:DT:H73	8:W:158:ARG:NH1	1.70	1.06
2:3:17:DG:C5	5:O:567:PHE:CE2	2.44	1.06
4:I:191:ARG:NH2	4:J:243:ARG:HH22	1.44	1.06
4:D:84:GLY:HA3	4:J:194:LEU:HD11	1.36	1.05
4:E:211:TRP:HZ2	4:E:241:ILE:HD11	1.22	1.05
4:J:53:ARG:HG2	4:K:29:LYS:NZ	1.56	1.04
8:W:360:GLU:OE1	8:Y:521:LYS:NZ	1.89	1.04
1:1:-24:DC:H5	8:W:77:ARG:NH1	1.45	1.04
4:C:211:TRP:CE3	4:C:215:VAL:HG21	1.93	1.04
8:W:352:LYS:O	8:Y:524:LYS:HD2	1.56	1.04
4:A:116:ARG:CD	4:F:184:GLU:CD	2.31	1.04
4:F:185:GLN:OE1	4:G:173:THR:HG21	1.55	1.04
4:K:185:GLN:OE1	4:L:62:SER:HB3	1.57	1.04
8:W:322:ARG:NH1	11:5:4:DA:N3	2.03	1.04
4:K:85:ARG:HB2	4:K:86:PRO:CD	1.89	1.03
4:K:185:GLN:OE1	4:L:173:THR:HG21	1.58	1.03
8:X:380:ARG:NH1	9:2:3:DT:H3'	1.74	1.03
4:B:126:ARG:NH1	4:C:97:HIS:CG	2.26	1.03
6:Q:149:GLY:C	6:Q:158:PHE:CD1	2.36	1.03
4:K:85:ARG:HB2	4:K:86:PRO:HD2	1.04	1.02
4:H:264:ASP:OD2	4:H:267:VAL:HG12	1.60	1.01
1:1:42:DC:H5''	4:L:119:LYS:HD2	1.43	1.01
2:3:-2:DT:O3'	5:O:414:THR:HG21	1.60	1.01
5:O:292:VAL:HB	5:O:304:HIS:NE2	1.73	1.01
8:X:425:GLN:HB3	12:6:12:DC:OP1	1.60	1.01
2:3:-5:DT:P	5:O:309:SER:OG	2.18	1.01
4:E:220:VAL:HG12	4:E:262:LYS:HD3	1.43	1.00
4:F:116:ARG:N	4:L:174:ASP:OD2	1.93	1.00
1:1:42:DC:H5'	4:L:119:LYS:HD2	1.43	1.00
8:W:306:PHE:O	8:W:306:PHE:CD1	2.15	1.00
5:O:412:SER:CB	5:O:415:GLN:OE1	2.10	0.99
1:1:36:DG:H3'	4:I:119:LYS:HE2	0.99	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:141:LEU:HD11	4:A:168:VAL:CG1	1.91	0.99
8:x:576:GLU:CG	8:x:579:ARG:HH22	1.71	0.99
4:F:218:LEU:HD22	4:F:256:LEU:HD21	1.01	0.99
4:J:53:ARG:HG3	4:K:29:LYS:HZ1	1.25	0.99
4:K:85:ARG:CB	4:K:86:PRO:HD2	1.93	0.98
4:L:115:TYR:CE1	6:Q:155:ARG:HD3	1.97	0.98
8:X:355:ARG:HE	8:Z:522:SER:HA	1.29	0.98
1:1:-2:DC:H1'	8:X:321:GLU:O	1.64	0.98
4:F:218:LEU:CD2	4:F:256:LEU:CD1	2.31	0.98
2:3:-5:DT:OP2	5:O:309:SER:OG	1.81	0.98
8:Y:523:ARG:HG3	8:Y:526:ARG:NE	1.77	0.98
2:3:17:DG:C6	5:O:567:PHE:CE2	2.50	0.98
4:B:185:GLN:OE1	4:C:173:THR:HG21	1.64	0.98
1:1:42:DC:C5'	4:L:119:LYS:CD	2.41	0.98
4:I:207:THR:HG22	4:I:211:TRP:HE1	1.28	0.98
1:1:50:DA:H5''	5:O:275:ARG:HG2	1.45	0.97
2:3:-1:DT:OP1	5:O:414:THR:CB	2.13	0.97
4:I:254:ARG:HD2	4:I:267:VAL:HG13	1.45	0.97
8:W:203:GLN:HB2	8:W:320:VAL:CG2	1.95	0.97
6:Q:149:GLY:C	6:Q:158:PHE:HD1	1.70	0.96
4:C:116:ARG:N	4:I:174:ASP:OD2	1.97	0.96
5:O:292:VAL:CG1	5:O:304:HIS:NE2	2.28	0.96
4:J:82:GLU:CD	4:J:85:ARG:HD2	1.91	0.96
2:3:-1:DT:O3'	5:O:418:LEU:CD1	2.14	0.95
4:H:85:ARG:CG	4:H:86:PRO:HD2	1.94	0.95
4:K:20:TRP:HZ3	4:K:21:LEU:HD23	1.28	0.95
8:X:178:TRP:HA	9:2:1:DT:O2	1.66	0.95
4:L:20:TRP:CZ3	4:L:21:LEU:HD23	2.02	0.95
1:1:-12:DT:C7	8:W:158:ARG:NH1	2.30	0.95
4:J:82:GLU:CG	4:J:85:ARG:HD2	1.96	0.94
8:W:380:ARG:NH1	11:5:3:DT:OP1	1.63	0.94
4:H:185:GLN:NE2	4:I:62:SER:HB2	1.82	0.94
4:I:191:ARG:HE	4:J:243:ARG:HH21	1.12	0.94
4:A:116:ARG:HD2	4:F:184:GLU:CD	1.92	0.94
4:H:185:GLN:NE2	4:I:62:SER:CB	2.30	0.94
5:O:478:LYS:CG	5:O:485:TYR:CE2	2.50	0.94
4:K:28:LEU:O	4:K:249:ARG:NH1	2.01	0.94
1:1:42:DC:H4'	4:L:119:LYS:HD3	1.49	0.94
5:O:17:ARG:NH1	5:O:371:LEU:HB2	1.81	0.93
4:E:220:VAL:CG1	4:E:262:LYS:HD3	1.99	0.93
8:X:380:ARG:HH12	9:2:3:DT:C3'	1.82	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:67:THR:HG1	13:G:301:MG:MG	0.70	0.92
4:G:158:ARG:HD2	4:G:189:ARG:HH12	1.24	0.92
5:O:17:ARG:NH1	5:O:371:LEU:HD12	1.84	0.92
4:F:211:TRP:HZ2	4:F:241:ILE:HD11	1.33	0.92
4:H:85:ARG:HG2	4:H:86:PRO:HD2	1.49	0.92
4:E:211:TRP:CZ2	4:E:241:ILE:HD11	2.04	0.92
14:B:302:ATP:H5'1	14:B:302:ATP:H8	1.32	0.92
4:J:53:ARG:CB	4:K:29:LYS:HE3	1.99	0.91
4:I:207:THR:O	4:I:211:TRP:CD1	2.23	0.91
4:J:53:ARG:HB2	4:K:29:LYS:HE3	1.52	0.91
4:B:185:GLN:OE1	4:C:62:SER:HB3	1.71	0.91
1:1:42:DC:C4'	4:L:119:LYS:NZ	2.33	0.91
3:7:186:A:P	5:O:362:LYS:HE3	2.10	0.91
8:X:136:LEU:HD22	8:Y:508:GLN:OE1	1.71	0.91
1:1:-8:DA:OP2	8:Z:495:ARG:HD3	1.70	0.91
4:K:185:GLN:NE2	4:L:62:SER:HB2	1.86	0.90
1:1:36:DG:H5'	4:I:119:LYS:NZ	1.87	0.90
4:D:99:LYS:HB3	4:D:150:LYS:NZ	1.86	0.90
8:X:293:ARG:HH22	12:6:19:DT:H5''	1.36	0.90
4:I:121:THR:HG22	4:I:124:ASP:OD2	1.71	0.90
4:H:184:GLU:OE2	4:I:61:GLU:OE2	1.90	0.90
4:A:141:LEU:O	4:A:141:LEU:HD12	1.71	0.90
8:W:153:TYR:OH	9:2:7:DG:OP2	1.90	0.90
4:K:28:LEU:HD13	4:K:253:ILE:HG13	1.54	0.90
4:A:141:LEU:HD21	4:A:168:VAL:HG22	1.54	0.89
8:W:353:ASP:HA	8:Y:524:LYS:CD	2.00	0.89
3:7:229:A:N7	5:O:320:ARG:NH1	2.20	0.89
5:O:35:LEU:O	5:O:39:LEU:HG	1.72	0.89
4:I:145:GLU:HB3	4:I:148:ARG:HD2	1.53	0.89
4:I:191:ARG:CZ	4:J:243:ARG:HH22	1.64	0.89
8:X:495:ARG:NE	12:6:13:DT:H5'	1.87	0.88
4:K:20:TRP:CE3	4:K:21:LEU:HD23	2.08	0.88
5:O:292:VAL:CB	5:O:304:HIS:NE2	2.35	0.88
3:7:55:A:C2	5:O:497:TYR:HB2	2.08	0.88
4:K:202:GLU:OE1	4:K:202:GLU:N	2.07	0.88
5:O:478:LYS:HG2	5:O:485:TYR:CD2	2.09	0.88
8:X:155:THR:HG21	10:4:-12:DA:H3'	1.54	0.88
5:O:355:VAL:CG1	5:O:374:TYR:HE2	1.84	0.88
8:Y:523:ARG:CG	8:Y:526:ARG:HE	1.87	0.88
3:7:41:A:P	5:O:478:LYS:HE3	2.14	0.87
8:W:178:TRP:CE3	11:5:1:DT:C4	2.63	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:81:ARG:NH1	9:2:20:DT:H73	1.90	0.87
4:C:211:TRP:HZ3	4:C:215:VAL:HG21	1.39	0.87
8:x:576:GLU:CB	8:x:579:ARG:NH2	2.37	0.87
8:W:352:LYS:O	8:Y:524:LYS:CD	2.22	0.87
1:1:-24:DC:C6	8:W:77:ARG:CZ	2.54	0.87
4:F:218:LEU:CD2	4:F:256:LEU:HD21	1.97	0.86
4:I:254:ARG:HD2	4:I:267:VAL:CG1	2.04	0.86
1:1:60:DC:H2''	5:O:351:ASN:CG	2.00	0.86
3:7:165:G:N2	7:S:22:THR:OG1	2.07	0.86
3:7:186:A:OP1	5:O:362:LYS:HE3	1.75	0.86
8:W:75:SER:N	9:2:21:DG:OP2	2.09	0.86
1:1:30:DC:H2''	1:1:31:DA:C8	2.11	0.85
3:7:41:A:OP1	5:O:478:LYS:HB2	1.76	0.85
8:X:425:GLN:C	12:6:12:DC:OP1	2.19	0.85
4:H:85:ARG:CG	4:H:86:PRO:CD	2.55	0.84
5:O:39:LEU:HD23	5:O:91:TYR:HH	1.36	0.84
4:I:207:THR:O	4:I:211:TRP:HD1	1.57	0.84
8:x:576:GLU:HG3	8:x:579:ARG:HH22	1.02	0.84
4:F:211:TRP:CZ2	4:F:241:ILE:HD11	2.12	0.84
8:W:81:ARG:NH1	9:2:20:DT:C7	2.41	0.84
8:X:246:ALA:HB3	10:4:7:DT:OP1	1.77	0.84
5:O:292:VAL:CG2	5:O:304:HIS:CE1	2.61	0.84
4:L:115:TYR:CZ	6:Q:155:ARG:HD3	2.13	0.83
4:I:191:ARG:CZ	4:J:243:ARG:HH21	1.56	0.83
5:O:42:HIS:HE1	5:O:44:ASP:HB2	0.73	0.83
4:I:207:THR:HG22	4:I:211:TRP:NE1	1.93	0.83
8:W:352:LYS:O	8:Y:524:LYS:CG	2.27	0.83
1:1:-1:DA:C2	8:X:314:PRO:O	2.30	0.83
4:I:211:TRP:CZ2	4:I:241:ILE:CD1	2.51	0.83
8:W:341:SER:HB2	10:4:-2:DC:OP1	1.78	0.83
4:C:185:GLN:OE1	4:D:62:SER:HB3	1.79	0.82
4:L:250:GLU:OE2	4:L:275:TYR:OH	1.96	0.82
4:H:185:GLN:CD	4:I:62:SER:HB3	2.04	0.82
8:W:346:ARG:HD3	10:4:2:DT:H72	1.60	0.82
8:X:235:ARG:HD2	9:2:4:DA:OP1	1.79	0.82
8:X:495:ARG:NH1	12:6:13:DT:H3'	1.95	0.82
1:1:42:DC:H4'	4:L:119:LYS:CD	2.10	0.81
4:K:185:GLN:CD	4:L:62:SER:HB3	2.03	0.81
1:1:42:DC:C4'	4:L:119:LYS:HZ2	1.92	0.81
4:D:211:TRP:CE3	4:D:215:VAL:HG21	2.15	0.81
4:K:79:PRO:HG2	6:Q:5:PRO:HB2	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:42:HIS:CE1	5:O:44:ASP:CB	2.48	0.81
8:W:353:ASP:HA	8:Y:524:LYS:HD3	1.60	0.81
4:C:99:LYS:O	4:C:150:LYS:HE3	1.81	0.81
4:D:99:LYS:O	4:D:150:LYS:HE2	1.80	0.81
5:O:412:SER:CB	5:O:415:GLN:CG	2.59	0.80
8:X:58:ARG:NH2	10:4:-27:DC:C2	2.48	0.80
14:B:302:ATP:H5'1	14:B:302:ATP:C8	2.15	0.80
4:K:185:GLN:HE22	4:L:62:SER:HB2	1.43	0.80
1:I:136:DG:C4'	4:I:119:LYS:HE2	2.12	0.80
4:L:20:TRP:HZ3	4:L:21:LEU:HD23	1.45	0.79
3:7:246:A:OP1	7:S:65:LYS:HE3	1.82	0.79
8:x:576:GLU:CB	8:x:579:ARG:HH21	1.94	0.79
4:I:254:ARG:CD	4:I:267:VAL:HG13	2.11	0.79
4:K:20:TRP:HZ3	4:K:21:LEU:CD2	1.95	0.79
4:H:99:LYS:O	4:H:150:LYS:HE3	1.83	0.79
4:J:82:GLU:OE2	4:J:85:ARG:HD2	1.82	0.79
4:E:185:GLN:OE1	4:F:173:THR:HG21	1.81	0.79
8:W:178:TRP:CE3	11:5:1:DT:O4	2.36	0.79
4:C:211:TRP:CD1	4:C:244:LEU:CD2	2.65	0.79
4:E:99:LYS:O	4:E:150:LYS:HE3	1.83	0.78
4:I:207:THR:CG2	4:I:211:TRP:HE1	1.95	0.78
4:K:150:LYS:HG2	4:K:151:PRO:HD2	1.66	0.78
8:X:106:ARG:NH1	10:4:-13:DT:O4'	2.17	0.78
5:O:478:LYS:HG2	5:O:485:TYR:CZ	2.18	0.78
4:G:99:LYS:O	4:G:150:LYS:HE3	1.83	0.78
5:O:418:LEU:HG	5:O:421:ARG:NH2	1.99	0.78
3:7:87:C:N3	5:O:321:GLN:OE1	2.17	0.78
3:7:239:A:H5'	5:O:586:HIS:NE2	1.99	0.78
8:W:360:GLU:CD	8:Y:521:LYS:NZ	2.41	0.78
4:I:185:GLN:NE2	4:I:189:ARG:HH12	1.82	0.78
5:O:81:MET:C	5:O:85:HIS:HD1	1.90	0.78
8:W:230:ILE:CG2	8:W:320:VAL:HG22	2.13	0.78
4:C:211:TRP:CE3	4:C:215:VAL:CG2	2.67	0.77
4:C:211:TRP:HD1	4:C:244:LEU:HD21	1.48	0.77
4:K:185:GLN:NE2	4:K:189:ARG:HH12	1.82	0.77
4:A:116:ARG:HD2	4:F:184:GLU:OE2	1.83	0.77
4:H:85:ARG:HG3	4:H:86:PRO:HD2	1.65	0.77
4:K:185:GLN:OE1	4:L:173:THR:CG2	2.32	0.77
8:X:106:ARG:NH1	10:4:-13:DT:C4'	2.48	0.77
8:Z:502:SER:O	8:Z:504:GLN:HG2	1.84	0.77
1:I:30:DC:H2''	1:I:31:DA:H8	1.46	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:50:ARG:HD2	4:A:139:GLU:HB2	1.66	0.77
4:H:85:ARG:HG3	4:H:86:PRO:CD	2.14	0.77
8:W:203:GLN:HB2	8:W:320:VAL:HG21	1.65	0.77
4:C:54:LYS:HE2	4:D:246:GLU:HG3	1.67	0.77
4:C:211:TRP:CZ3	4:C:215:VAL:CG2	2.63	0.77
4:F:99:LYS:O	4:F:150:LYS:HE3	1.83	0.77
4:A:116:ARG:CD	4:F:184:GLU:OE2	2.33	0.77
2:3:-1:DT:H1'	5:O:418:LEU:HD12	1.66	0.77
4:K:20:TRP:CZ3	4:K:21:LEU:CD2	2.66	0.77
4:A:141:LEU:CD2	4:A:168:VAL:HG22	2.15	0.76
5:O:355:VAL:CG1	5:O:374:TYR:CE2	2.68	0.76
5:O:292:VAL:HG21	5:O:304:HIS:HE1	1.50	0.76
1:1:57:DT:O2	5:O:93:SER:OG	2.03	0.76
4:H:85:ARG:HG2	4:H:86:PRO:CD	2.16	0.76
4:K:28:LEU:HD13	4:K:253:ILE:CG1	2.15	0.76
5:O:39:LEU:HD21	5:O:91:TYR:OH	1.86	0.76
8:X:99:ARG:NH1	11:5:16:DT:O2	2.18	0.76
4:J:82:GLU:OE2	4:J:85:ARG:CD	2.34	0.75
4:K:150:LYS:CG	4:K:151:PRO:HD2	2.16	0.75
1:1:42:DC:H5''	4:L:119:LYS:CD	2.08	0.75
4:B:126:ARG:HD3	4:C:97:HIS:CE1	2.21	0.75
4:I:211:TRP:HZ2	4:I:241:ILE:HD11	0.73	0.75
4:I:185:GLN:HE21	4:I:189:ARG:HH12	1.35	0.75
8:W:346:ARG:CD	10:4:2:DT:H72	2.16	0.75
3:7:41:A:OP2	5:O:478:LYS:HE3	1.87	0.75
1:1:31:DA:H1'	1:1:32:DA:C8	2.22	0.75
4:K:131:GLU:OE1	6:Q:34:HIS:NE2	2.20	0.75
5:O:412:SER:O	5:O:416:GLN:HG2	1.87	0.74
8:X:155:THR:CG2	10:4:-12:DA:H2'	2.17	0.74
5:O:9:ARG:HH21	5:O:370:HIS:HD2	1.35	0.74
4:E:211:TRP:HZ2	4:E:241:ILE:CD1	1.99	0.74
4:F:134:LYS:HE3	4:F:164:LEU:HD21	1.68	0.74
5:O:31:LEU:HD23	5:O:281:PHE:CD1	2.22	0.74
8:X:178:TRP:HD1	9:2:3:DT:P	2.10	0.74
4:B:185:GLN:OE1	4:C:173:THR:CG2	2.36	0.74
4:J:20:TRP:CZ3	4:J:21:LEU:HD23	2.22	0.74
4:B:185:GLN:CD	4:C:173:THR:HG21	2.12	0.74
4:H:185:GLN:HE21	4:H:189:ARG:HH12	1.32	0.74
4:B:152:GLU:HG2	4:C:99:LYS:HE2	1.69	0.73
5:O:42:HIS:NE2	5:O:48:TRP:CZ2	2.57	0.73
8:W:81:ARG:HH12	9:2:20:DT:C7	2.01	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:42:DC:C4'	4:L:119:LYS:CD	2.65	0.73
5:O:81:MET:HB3	5:O:85:HIS:HE1	1.53	0.73
4:D:65:GLY:HA2	14:D:302:ATP:O2A	1.88	0.73
5:O:31:LEU:HD23	5:O:281:PHE:CG	2.23	0.73
8:X:178:TRP:N	9:2:3:DT:OP2	2.14	0.73
3:7:49:U:H4'	3:7:50:A:OP2	1.88	0.73
4:F:131:GLU:OE1	4:L:181:LYS:CE	2.35	0.73
4:H:185:GLN:NE2	4:H:189:ARG:HH12	1.85	0.73
8:X:246:ALA:HB3	10:4:7:DT:P	2.27	0.73
5:O:27:LEU:O	5:O:31:LEU:HD13	1.88	0.73
2:3:21:DA:H5''	4:L:122:VAL:HG23	1.69	0.73
4:F:152:GLU:HB2	4:G:98:GLN:HG2	1.69	0.73
4:L:116:ARG:HG2	6:Q:147:GLU:OE1	1.89	0.73
8:W:318:GLY:HA2	11:5:2:DG:H21	1.52	0.73
2:3:48:DA:OP1	8:W:495:ARG:NE	2.21	0.73
4:B:185:GLN:OE1	4:C:62:SER:CB	2.36	0.73
5:O:292:VAL:CG2	5:O:304:HIS:HE1	2.03	0.72
8:X:380:ARG:NH1	9:2:4:DA:OP2	2.22	0.72
4:C:211:TRP:CD1	4:C:244:LEU:HD21	2.25	0.72
8:Z:519:THR:HA	8:Z:522:SER:HB2	1.71	0.72
4:F:211:TRP:CE3	4:F:215:VAL:HG21	2.23	0.72
4:H:65:GLY:HA2	14:H:302:ATP:O2A	1.89	0.72
3:7:241:U:P	5:O:579:LYS:HZ1	2.11	0.72
3:7:234:A:OP1	5:O:240:ARG:NH2	2.18	0.72
4:K:65:GLY:HA2	14:K:302:ATP:O2A	1.90	0.72
4:K:185:GLN:HE21	4:K:189:ARG:HH12	1.35	0.72
4:C:65:GLY:HA2	14:C:302:ATP:O2A	1.89	0.72
4:E:65:GLY:HA2	14:E:302:ATP:O2A	1.90	0.71
8:W:346:ARG:HD3	10:4:2:DT:C7	2.20	0.71
3:7:241:U:P	5:O:579:LYS:NZ	2.64	0.71
8:X:318:GLY:HA2	9:2:2:DG:N2	2.05	0.71
4:D:99:LYS:HB3	4:D:150:LYS:HZ1	1.56	0.71
8:X:246:ALA:CB	10:4:7:DT:P	2.78	0.71
4:C:116:ARG:NE	4:H:184:GLU:OE1	2.23	0.71
4:K:185:GLN:NE2	4:L:62:SER:CB	2.53	0.71
8:X:318:GLY:HA2	9:2:2:DG:H21	1.56	0.71
4:B:126:ARG:CD	4:C:97:HIS:CE1	2.74	0.71
8:X:78:THR:HG23	11:5:20:DT:OP2	1.92	0.70
8:X:427:GLN:NE2	8:X:488:GLU:OE2	2.24	0.70
2:3:27:DT:H1'	2:3:28:DT:H5''	1.73	0.70
5:O:292:VAL:HG11	5:O:304:HIS:NE2	2.04	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:X:155:THR:HG21	10:4:-12:DA:C3'	2.22	0.70
3:7:104:C:O2'	7:S:42:HIS:CD2	2.45	0.70
1:1:36:DG:C5'	4:I:119:LYS:CE	2.70	0.70
3:7:87:C:C2	5:O:321:GLN:OE1	2.45	0.70
4:A:116:ARG:HD3	4:F:184:GLU:CD	2.14	0.70
1:1:32:DA:C6	1:1:33:DA:C6	2.80	0.70
1:1:-24:DC:C6	8:W:77:ARG:NH1	2.56	0.69
2:3:-1:DT:P	5:O:414:THR:HG21	2.32	0.69
4:J:150:LYS:HE2	4:J:152:GLU:OE2	1.92	0.69
5:O:31:LEU:CD2	5:O:281:PHE:CD1	2.76	0.69
3:7:41:A:OP1	5:O:478:LYS:HE3	1.92	0.69
1:1:33:DA:H2''	1:1:34:DT:OP2	1.92	0.69
4:G:67:THR:OG1	13:G:301:MG:MG	1.36	0.69
4:K:189:ARG:NH2	14:L:302:ATP:O1G	2.25	0.69
8:X:106:ARG:NH1	10:4:-13:DT:H4'	2.08	0.69
1:1:50:DA:H2'	1:1:51:DA:C8	2.28	0.69
4:H:155:ALA:HB1	4:I:148:ARG:HH21	1.58	0.69
4:K:85:ARG:CB	4:K:86:PRO:CD	2.62	0.69
8:W:230:ILE:HG22	8:W:320:VAL:HG22	1.74	0.69
4:J:53:ARG:CG	4:K:29:LYS:HZ1	1.84	0.68
4:E:207:THR:HG22	4:E:211:TRP:HE1	1.58	0.68
6:Q:149:GLY:O	6:Q:158:PHE:HD1	1.75	0.68
8:X:155:THR:HG22	10:4:-12:DA:H2'	1.74	0.68
8:X:318:GLY:CA	9:2:2:DG:H21	2.06	0.68
1:1:35:DT:O3'	4:I:119:LYS:NZ	2.25	0.68
8:X:425:GLN:HB2	12:6:12:DC:OP1	1.94	0.68
4:K:112:TYR:CZ	6:Q:5:PRO:HG3	2.28	0.68
4:D:99:LYS:HB3	4:D:150:LYS:HZ3	1.58	0.68
4:G:65:GLY:HA2	14:G:302:ATP:O2A	1.94	0.68
4:A:141:LEU:CG	4:A:168:VAL:HG22	2.24	0.68
1:1:35:DT:H4'	1:1:36:DG:OP1	1.94	0.68
4:K:112:TYR:OH	6:Q:5:PRO:HG3	1.93	0.68
7:S:45:GLU:HG2	7:S:46:HIS:HD2	1.58	0.68
8:X:158:ARG:NH1	10:4:-12:DA:C8	2.62	0.68
4:F:65:GLY:HA2	14:F:302:ATP:O2A	1.94	0.67
8:X:155:THR:CG2	10:4:-12:DA:C2'	2.72	0.67
8:X:246:ALA:HB1	10:4:6:DA:O3'	1.93	0.67
4:F:218:LEU:HD11	4:F:252:ALA:HB1	1.76	0.67
3:7:23:U:O4	5:O:620:HIS:CE1	2.48	0.67
4:F:218:LEU:HD21	4:F:256:LEU:HD11	0.70	0.67
8:X:318:GLY:HA3	9:2:2:DG:N3	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:185:GLN:OE1	4:G:173:THR:CG2	2.38	0.67
8:W:75:SER:HB3	9:2:21:DG:OP2	1.95	0.67
4:I:185:GLN:OE1	4:J:62:SER:HB3	1.93	0.67
8:W:178:TRP:HE3	11:5:1:DT:O4	1.78	0.67
8:x:576:GLU:HG3	8:x:579:ARG:CZ	2.19	0.67
1:1:53:DG:OP1	5:O:517:SER:OG	2.10	0.67
4:B:99:LYS:O	4:B:150:LYS:HE3	1.95	0.67
8:W:203:GLN:CB	8:W:320:VAL:HG21	2.25	0.66
3:7:125:U:H3	3:7:132:A:H61	1.42	0.66
4:K:185:GLN:CD	4:L:62:SER:CB	2.67	0.66
4:F:218:LEU:HD22	4:F:256:LEU:CG	2.26	0.66
4:E:66:LYS:NZ	14:E:302:ATP:O2G	2.25	0.66
1:1:42:DC:C4'	4:L:119:LYS:HZ3	2.08	0.66
4:B:126:ARG:NH1	4:C:97:HIS:CD2	2.64	0.66
4:G:185:GLN:HE21	4:G:185:GLN:HA	1.61	0.66
8:W:178:TRP:HD1	11:5:3:DT:P	2.18	0.66
1:1:1:DT:O3'	8:X:223:ARG:NH2	2.29	0.66
4:A:189:ARG:NH1	14:B:302:ATP:O3G	2.26	0.66
4:E:207:THR:HG22	4:E:211:TRP:NE1	2.11	0.66
8:W:39:SER:O	8:W:43:GLN:HG2	1.95	0.66
4:A:144:ASP:OD1	4:A:145:GLU:N	2.27	0.65
4:J:53:ARG:HG2	4:K:29:LYS:CE	2.06	0.65
4:L:20:TRP:CE3	4:L:21:LEU:HD23	2.31	0.65
8:x:576:GLU:HB2	8:x:579:ARG:HH21	1.60	0.65
14:D:302:ATP:H5'1	14:D:302:ATP:H8	1.61	0.65
3:7:246:A:OP1	7:S:65:LYS:CE	2.45	0.65
3:7:86:G:C2	5:O:300:ARG:NH2	2.31	0.65
4:A:93:TYR:HD1	4:A:142:ILE:CG2	2.10	0.65
1:1:8:DT:H2'	1:1:9:DA:C8	2.32	0.65
3:7:55:A:N6	3:7:145:G:O2'	2.29	0.65
3:7:203:C:O4'	5:O:11:ILE:HD12	1.97	0.65
4:J:74:ARG:HD3	4:J:93:TYR:HB3	1.78	0.65
8:X:293:ARG:HH22	12:6:19:DT:C5'	2.09	0.65
2:3:-1:DT:OP1	5:O:414:THR:CG2	2.44	0.65
4:A:67:THR:OG1	13:A:301:MG:MG	1.40	0.65
2:3:-1:DT:HO3'	5:O:418:LEU:HD13	1.61	0.64
4:K:79:PRO:CG	6:Q:5:PRO:HB2	2.26	0.64
5:O:446:HIS:CE1	5:O:447:ILE:HG13	2.32	0.64
3:7:229:A:C5	5:O:320:ARG:NH1	2.62	0.64
8:W:353:ASP:HA	8:Y:524:LYS:HD2	1.78	0.64
2:3:27:DT:H4'	2:3:28:DT:OP1	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:7:240:U:HO2'	3:7:241:U:H6	1.46	0.64
8:W:58:ARG:HA	8:W:61:TYR:HD2	1.61	0.64
4:B:158:ARG:HD2	4:B:189:ARG:HD2	1.79	0.64
1:1:-12:DT:C5	8:W:158:ARG:NH1	2.66	0.64
2:3:38:DA:H1'	2:3:39:DT:H5'	1.80	0.64
3:7:169:G:H5''	6:Q:128:LYS:HD3	1.79	0.64
1:1:35:DT:H1'	1:1:36:DG:H5''	1.79	0.64
4:A:93:TYR:HD1	4:A:142:ILE:HB	1.62	0.64
4:F:211:TRP:HE1	4:F:244:LEU:HD23	1.63	0.64
4:I:145:GLU:CB	4:I:148:ARG:HD2	2.28	0.64
8:W:215:ASP:O	8:Y:523:ARG:NH1	2.30	0.64
8:W:427:GLN:O	8:W:428:ASN:HB2	1.95	0.64
4:D:84:GLY:O	4:J:194:LEU:HD12	1.98	0.64
4:D:84:GLY:CA	4:J:194:LEU:HD11	2.22	0.64
1:1:47:DT:O2	5:O:266:LYS:HE3	1.98	0.64
2:3:21:DA:OP1	4:L:121:THR:OG1	2.15	0.64
4:H:185:GLN:CD	4:I:62:SER:CB	2.68	0.64
1:1:-17:DT:H2''	1:1:-16:DA:C8	2.33	0.63
4:B:126:ARG:NH1	4:C:97:HIS:CB	2.62	0.63
4:J:82:GLU:CD	4:J:85:ARG:CD	2.69	0.63
5:O:42:HIS:CE1	5:O:48:TRP:CZ2	2.86	0.63
8:W:352:LYS:C	8:Y:524:LYS:HD2	2.24	0.63
4:C:211:TRP:CD1	4:C:244:LEU:HG	2.34	0.63
8:Y:281:PRO:HB2	8:Y:283:HIS:O	1.98	0.63
4:F:211:TRP:CZ3	4:F:215:VAL:HG21	2.33	0.63
4:G:152:GLU:HB2	4:H:98:GLN:HG2	1.81	0.63
4:G:158:ARG:CG	4:G:189:ARG:HH11	2.10	0.63
5:O:355:VAL:HG12	5:O:374:TYR:CE2	2.34	0.63
4:A:93:TYR:CD1	4:A:142:ILE:CG2	2.81	0.63
6:Q:150:CYS:N	6:Q:158:PHE:CE1	2.66	0.63
1:1:-12:DT:H73	8:W:158:ARG:CZ	2.29	0.63
1:1:46:DA:H2'	1:1:47:DT:H71	1.80	0.62
4:F:134:LYS:CE	4:F:164:LEU:HD21	2.27	0.62
4:I:65:GLY:HA2	14:I:302:ATP:O2A	1.99	0.62
8:W:360:GLU:OE2	8:Y:521:LYS:HE2	1.98	0.62
3:7:48:U:H1'	4:H:85:ARG:HD3	1.80	0.62
4:A:141:LEU:HD21	4:A:168:VAL:CG2	2.29	0.62
5:O:478:LYS:CD	5:O:485:TYR:CE2	2.82	0.62
8:X:425:GLN:CA	12:6:12:DC:OP1	2.47	0.62
4:F:228:GLU:OE1	4:F:228:GLU:N	2.24	0.62
4:I:191:ARG:HH21	4:J:243:ARG:NH2	1.93	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:112:TYR:CZ	6:Q:5:PRO:CG	2.83	0.62
4:D:184:GLU:HG2	8:W:432:ARG:NH2	2.14	0.62
1:1:50:DA:H2'	1:1:51:DA:H8	1.63	0.62
2:3:34:DC:H2'	2:3:35:DT:H72	1.79	0.62
8:X:158:ARG:NH1	10:4:-12:DA:N7	2.47	0.62
4:B:126:ARG:CZ	4:C:97:HIS:CG	2.82	0.62
4:D:228:GLU:OE1	4:D:228:GLU:N	2.23	0.62
4:K:28:LEU:CD1	4:K:253:ILE:CG1	2.77	0.62
1:1:62:DA:C8	5:O:287:THR:HG23	2.35	0.62
4:G:158:ARG:HG2	4:G:189:ARG:HD2	1.80	0.62
5:O:355:VAL:HG11	5:O:374:TYR:CE2	2.35	0.62
3:7:239:A:H2'	3:7:240:U:C6	2.35	0.62
4:F:67:THR:OG1	13:F:301:MG:MG	1.43	0.62
5:O:17:ARG:HH12	5:O:371:LEU:CB	1.94	0.62
2:3:34:DC:H2'	2:3:35:DT:C7	2.30	0.61
4:J:264:ASP:OD1	4:J:265:LYS:N	2.31	0.61
8:W:131:PRO:HD2	9:2:7:DG:OP1	2.00	0.61
3:7:54:G:O2'	3:7:144:C:O2'	2.17	0.61
4:C:211:TRP:HE1	4:C:244:LEU:HD23	1.65	0.61
1:1:48:DT:H1'	5:O:270:ASP:OD1	1.99	0.61
8:X:290:LYS:HB3	10:4:8:DA:H1'	1.80	0.61
8:W:178:TRP:N	11:5:3:DT:OP2	2.34	0.61
1:1:32:DA:H1'	1:1:33:DA:H5'	1.81	0.61
4:A:82:GLU:OE2	4:H:273:LYS:NZ	2.34	0.61
4:B:158:ARG:CD	4:B:189:ARG:HD2	2.30	0.61
4:E:185:GLN:OE1	4:F:62:SER:HB3	2.01	0.61
6:Q:100:CYS:HB3	6:Q:103:CYS:SG	2.41	0.61
8:W:203:GLN:CB	8:W:320:VAL:CG2	2.76	0.61
1:1:59:DT:H4'	5:O:89:TYR:CE1	2.36	0.60
4:J:185:GLN:NE2	4:J:189:ARG:HH12	1.99	0.60
4:J:82:GLU:HG3	4:J:85:ARG:HD2	1.82	0.60
1:1:36:DG:C3'	4:I:119:LYS:CE	2.53	0.60
1:1:-14:DT:OP1	8:W:102:LYS:HD2	2.01	0.60
1:1:-11:DG:H2'	1:1:-10:DT:H71	1.83	0.60
2:3:46:DG:H2''	2:3:47:DC:H5''	1.83	0.60
5:O:31:LEU:HD22	5:O:281:PHE:HB2	1.83	0.60
5:O:478:LYS:CG	5:O:485:TYR:CZ	2.83	0.60
1:1:-12:DT:C7	8:W:158:ARG:CZ	2.79	0.60
1:1:36:DG:H1'	1:1:37:DA:C8	2.37	0.60
2:3:45:DC:H2''	2:3:46:DG:H5'	1.83	0.60
1:1:49:DA:H2''	1:1:50:DA:H5'	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:65:GLY:HA2	14:B:302:ATP:O3A	2.02	0.60
5:O:81:MET:HE3	5:O:85:HIS:CE1	2.36	0.60
6:Q:99:LEU:CD2	6:Q:158:PHE:HD2	2.15	0.60
8:X:58:ARG:NH2	10:4:-27:DC:H1'	2.17	0.60
6:Q:149:GLY:C	6:Q:158:PHE:CE1	2.79	0.59
3:7:232:A:H2'	3:7:233:G:H8	1.68	0.59
4:A:49:LYS:C	4:A:51:LYS:H	2.10	0.59
4:G:116:ARG:HG2	4:L:184:GLU:OE1	2.02	0.59
4:D:38:GLN:O	4:D:38:GLN:HG3	2.03	0.59
4:I:187:LEU:C	4:I:187:LEU:HD23	2.27	0.59
8:W:318:GLY:HA2	11:5:2:DG:N2	2.18	0.59
3:7:109:C:H2'	3:7:177:G:H22	1.66	0.59
5:O:31:LEU:CD2	5:O:281:PHE:CG	2.86	0.59
8:Z:463:ASN:O	8:Z:465:GLN:HG2	2.01	0.59
4:F:218:LEU:CD2	4:F:256:LEU:CG	2.80	0.59
8:Y:247:PRO:HA	8:Y:251:VAL:HG21	1.84	0.59
10:4:-17:DT:H2''	10:4:-16:DA:C8	2.37	0.59
1:1:42:DC:H4'	4:L:119:LYS:NZ	2.18	0.59
1:1:50:DA:C5'	5:O:275:ARG:HG2	2.27	0.59
4:J:20:TRP:CE3	4:J:21:LEU:HD23	2.37	0.59
5:O:42:HIS:CD2	5:O:48:TRP:CH2	2.91	0.59
8:X:142:ALA:HB2	8:X:150:PRO:HB3	1.85	0.59
1:1:11:DA:H5''	4:A:182:ARG:NH2	2.17	0.59
4:A:50:ARG:HG3	4:A:140:MET:HB2	1.85	0.59
4:K:28:LEU:CD1	4:K:253:ILE:HG12	2.32	0.59
3:7:238:C:O2'	3:7:239:A:H8	1.86	0.59
4:A:189:ARG:HH22	14:B:302:ATP:PG	2.26	0.59
4:C:126:ARG:HD3	4:D:97:HIS:CE1	2.37	0.58
4:C:131:GLU:OE1	4:I:181:LYS:NZ	2.21	0.58
4:I:185:GLN:HE22	4:J:62:SER:HB2	1.68	0.58
4:I:187:LEU:HD23	4:I:187:LEU:O	2.03	0.58
6:Q:13:LEU:CD1	6:Q:75:GLU:HB2	2.33	0.58
4:K:187:LEU:O	4:K:187:LEU:HD23	2.03	0.58
8:X:293:ARG:NH2	12:6:19:DT:H5''	2.14	0.58
8:X:495:ARG:HH11	12:6:13:DT:H3'	1.66	0.58
6:Q:149:GLY:O	6:Q:158:PHE:CD1	2.51	0.58
8:X:58:ARG:CG	10:4:-26:DA:H5'	2.33	0.58
8:X:99:ARG:NH1	10:4:-15:DA:C2	2.71	0.58
10:4:7:DT:H2'	10:4:8:DA:C8	2.38	0.58
4:K:187:LEU:HD23	4:K:187:LEU:C	2.28	0.58
5:O:355:VAL:HG11	5:O:374:TYR:HE2	1.65	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:126:ARG:NH2	4:C:97:HIS:HB3	2.18	0.58
8:X:178:TRP:CD2	9:2:1:DT:O2	2.55	0.58
1:1:32:DA:C2	1:1:33:DA:C4	2.91	0.58
5:O:292:VAL:CG1	5:O:304:HIS:CE1	2.82	0.58
8:Y:426:PHE:HA	10:4:-7:DC:OP1	2.04	0.58
8:W:343:VAL:CG2	10:4:2:DT:C4	2.87	0.58
8:X:178:TRP:CG	9:2:1:DT:O2	2.57	0.58
8:X:427:GLN:HE22	8:X:488:GLU:CD	2.11	0.58
5:O:81:MET:HB3	5:O:85:HIS:CE1	2.37	0.58
8:X:246:ALA:CB	10:4:6:DA:O3'	2.51	0.58
4:A:52:ALA:O	4:A:54:LYS:HG2	2.03	0.57
8:X:178:TRP:CA	9:2:1:DT:O2	2.48	0.57
4:B:126:ARG:CZ	4:C:97:HIS:HB3	2.34	0.57
4:G:158:ARG:HD2	4:G:189:ARG:HH11	0.76	0.57
5:O:31:LEU:CD2	5:O:281:PHE:HB2	2.33	0.57
5:O:355:VAL:HG12	5:O:374:TYR:HE2	1.64	0.57
2:3:48:DA:OP1	8:W:495:ARG:NH2	2.37	0.57
2:3:36:DA:H2''	2:3:37:DT:O5'	2.05	0.57
4:C:126:ARG:NH1	4:D:97:HIS:CG	2.72	0.57
4:L:62:SER:O	14:L:302:ATP:PG	2.63	0.57
11:5:21:DG:H2'	11:5:22:DT:H71	1.87	0.57
4:D:211:TRP:CZ3	4:D:215:VAL:HG21	2.40	0.57
4:A:141:LEU:HD12	4:A:141:LEU:C	2.29	0.57
4:K:188:GLU:HB3	4:L:63:ARG:HD2	1.86	0.57
6:Q:13:LEU:HD12	6:Q:74:VAL:O	2.05	0.57
8:x:576:GLU:HA	8:x:579:ARG:NH2	2.20	0.57
8:W:75:SER:CB	9:2:21:DG:OP2	2.52	0.57
8:X:136:LEU:CD2	8:Y:508:GLN:OE1	2.50	0.57
8:W:352:LYS:O	8:Y:524:LYS:HG3	2.05	0.57
4:D:117:VAL:HG11	4:D:125:PHE:CE2	2.40	0.57
4:G:116:ARG:HD2	4:L:184:GLU:HB3	1.86	0.57
5:O:292:VAL:HG21	5:O:304:HIS:CE1	2.31	0.57
4:K:105:LEU:HD22	4:K:153:THR:HG22	1.86	0.57
5:O:31:LEU:CD2	5:O:281:PHE:CB	2.83	0.57
1:1:2:DA:C6	8:X:343:VAL:CG2	2.88	0.56
4:D:84:GLY:HA3	4:J:194:LEU:CD1	2.24	0.56
1:1:61:DA:OP2	5:O:350:ARG:HB3	2.04	0.56
1:1:31:DA:C1'	1:1:32:DA:C8	2.89	0.56
3:7:41:A:OP2	5:O:478:LYS:CE	2.53	0.56
3:7:50:A:H2'	3:7:51:A:C8	2.40	0.56
4:A:116:ARG:HD2	4:F:184:GLU:OE1	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:19:GLU:O	4:H:22:GLN:HB3	2.06	0.56
5:O:16:ASN:OD1	5:O:311:LEU:HD22	2.06	0.56
8:W:346:ARG:CD	10:4:2:DT:C7	2.81	0.56
2:3:-1:DT:P	5:O:414:THR:CG2	2.93	0.56
4:E:220:VAL:HG11	4:E:262:LYS:HD3	1.87	0.56
4:J:187:LEU:HD23	4:J:187:LEU:C	2.30	0.56
8:X:293:ARG:HH21	12:6:19:DT:H4'	1.71	0.56
4:A:116:ARG:HD3	4:F:184:GLU:OE2	2.02	0.56
4:K:117:VAL:HG23	6:Q:11:LEU:CD2	2.36	0.56
3:7:54:G:O5'	5:O:493:ARG:NH1	2.39	0.56
4:C:211:TRP:CD1	4:C:244:LEU:CG	2.88	0.56
4:F:211:TRP:HE3	4:F:215:VAL:HG21	1.71	0.56
5:O:17:ARG:NH1	5:O:371:LEU:CD1	2.64	0.56
1:1:48:DT:H2'	1:1:49:DA:C8	2.40	0.56
4:B:103:LYS:HG3	4:B:122:VAL:HG22	1.88	0.56
8:X:303:GLN:HB3	8:X:408:ILE:HG21	1.86	0.56
4:H:266:ALA:O	4:H:270:GLU:HG3	2.05	0.56
4:J:187:LEU:HD23	4:J:187:LEU:O	2.06	0.56
8:Y:523:ARG:HG2	8:Y:523:ARG:O	2.06	0.56
1:1:2:DA:C5	8:X:343:VAL:HG23	2.41	0.55
4:A:93:TYR:HD1	4:A:142:ILE:CB	2.19	0.55
1:1:48:DT:H2''	5:O:270:ASP:OD1	2.06	0.55
4:J:20:TRP:HZ3	4:J:21:LEU:HD23	1.69	0.55
8:X:178:TRP:CE3	8:X:183:LEU:HA	2.41	0.55
2:3:29:DT:H1'	2:3:30:DG:O4'	2.07	0.55
9:2:3:DT:H2''	9:2:4:DA:C8	2.42	0.55
4:F:53:ARG:NH2	4:F:139:GLU:HG2	2.22	0.55
4:K:131:GLU:OE1	6:Q:34:HIS:CD2	2.60	0.55
5:O:14:GLU:O	5:O:15:SER:C	2.48	0.55
1:1:-14:DT:H5'	8:W:99:ARG:HD3	1.87	0.55
2:3:25:DA:H5''	4:J:122:VAL:HG21	1.89	0.55
8:W:81:ARG:HH11	9:2:20:DT:H73	1.67	0.55
11:5:3:DT:H2''	11:5:4:DA:C8	2.41	0.55
5:O:20:LEU:HD23	5:O:371:LEU:HD21	1.89	0.55
8:X:246:ALA:CB	10:4:7:DT:OP1	2.51	0.55
1:1:-14:DT:O2	8:W:106:ARG:NH1	2.40	0.55
6:Q:95:GLU:HB3	6:Q:96:PRO:HD3	1.89	0.55
11:5:11:DC:H2'	11:5:12:DT:H71	1.89	0.55
4:K:131:GLU:OE2	6:Q:32:ALA:O	2.25	0.55
8:X:178:TRP:CD1	9:2:3:DT:P	2.98	0.55
4:A:103:LYS:HG3	4:A:122:VAL:HG22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:65:GLY:HA2	14:B:302:ATP:PA	2.47	0.55
1:1:2:DA:C5	8:X:343:VAL:CG2	2.90	0.54
1:1:7:DA:C2	8:W:290:LYS:HG3	2.41	0.54
1:1:36:DG:C5'	4:I:119:LYS:HE2	2.35	0.54
4:C:211:TRP:HE3	4:C:215:VAL:HB	1.72	0.54
4:D:210:MET:HE3	8:y:570:ILE:HD11	1.88	0.54
8:Z:299:GLN:O	8:Z:300:ILE:C	2.51	0.54
3:7:232:A:H2'	3:7:233:G:C8	2.43	0.54
4:A:52:ALA:O	4:A:53:ARG:C	2.46	0.54
4:A:93:TYR:OH	4:A:144:ASP:HB2	2.07	0.54
4:L:20:TRP:HZ3	4:L:21:LEU:CD2	2.19	0.54
8:W:178:TRP:CD2	11:5:1:DT:C5	2.94	0.54
1:1:36:DG:H5'	4:I:119:LYS:CE	2.36	0.54
4:D:162:GLU:OE1	4:D:189:ARG:NH1	2.41	0.54
8:X:142:ALA:CB	8:X:150:PRO:HB3	2.37	0.54
1:1:48:DT:H4'	5:O:270:ASP:OD2	2.08	0.54
3:7:48:U:H5	3:7:50:A:C4	2.25	0.54
4:A:130:ILE:O	4:A:134:LYS:HG3	2.08	0.54
8:X:380:ARG:NH1	9:2:4:DA:P	2.81	0.54
8:Y:247:PRO:HA	8:Y:251:VAL:HG11	1.90	0.54
2:3:33:DT:H2''	2:3:34:DC:H6	1.73	0.54
4:B:126:ARG:HH11	4:C:97:HIS:CD2	2.26	0.54
6:Q:99:LEU:HD22	6:Q:158:PHE:CD2	2.42	0.54
4:I:99:LYS:O	4:I:150:LYS:HE3	2.08	0.54
5:O:14:GLU:OE2	5:O:367:ASN:ND2	2.38	0.54
8:W:306:PHE:O	8:W:306:PHE:CG	2.61	0.54
4:A:159:ASP:C	4:A:161:ALA:N	2.60	0.54
8:X:155:THR:HG21	10:4:-12:DA:C2'	2.38	0.54
8:X:318:GLY:CA	9:2:2:DG:N2	2.70	0.54
1:1:33:DA:C2'	1:1:34:DT:H71	2.38	0.53
4:A:133:LEU:HD22	4:A:166:ILE:HD13	1.90	0.53
5:O:13:PHE:HE1	5:O:15:SER:CB	2.00	0.53
6:Q:150:CYS:N	6:Q:158:PHE:CD1	2.75	0.53
8:X:426:PHE:O	8:X:427:GLN:C	2.48	0.53
4:K:28:LEU:CD1	4:K:253:ILE:HG13	2.34	0.53
4:K:28:LEU:HD12	4:K:253:ILE:HG12	1.89	0.53
8:W:203:GLN:HB2	8:W:320:VAL:HG23	1.87	0.53
3:7:66:G:H2'	3:7:67:A:H8	1.73	0.53
8:Y:434:GLU:OE2	8:Y:473:HIS:HE1	1.91	0.53
4:E:265:LYS:O	4:E:269:GLN:HG3	2.09	0.53
5:O:36:LEU:HD23	5:O:39:LEU:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:343:VAL:HG21	10:4:2:DT:C4	2.44	0.53
8:W:360:GLU:CD	8:Y:521:LYS:HZ1	2.14	0.53
4:F:128:ARG:HH11	4:L:181:LYS:NZ	2.06	0.53
8:X:106:ARG:HH11	10:4:-13:DT:H4'	1.71	0.53
8:X:290:LYS:HB3	10:4:8:DA:C1'	2.39	0.53
1:1:-12:DT:H73	8:W:158:ARG:HH11	1.69	0.53
3:7:9:A:N1	3:7:148:C:O2'	2.33	0.53
4:F:80:GLN:HB2	4:F:88:THR:OG1	2.07	0.53
4:J:97:HIS:O	4:J:148:ARG:HB3	2.08	0.53
6:Q:99:LEU:HD22	6:Q:158:PHE:HD2	1.72	0.53
1:1:62:DA:N7	5:O:287:THR:CG2	2.71	0.53
4:J:74:ARG:HD2	4:J:112:TYR:OH	2.08	0.53
10:4:-14:DT:H2'	10:4:-13:DT:H71	1.91	0.53
3:7:85:U:O2'	5:O:319:ASN:N	2.42	0.53
3:7:167:A:H5''	7:S:17:ARG:NH2	2.24	0.53
8:X:407:ASP:O	8:X:408:ILE:C	2.49	0.53
4:J:188:GLU:HB3	4:K:63:ARG:HD2	1.90	0.53
5:O:85:HIS:CD2	5:O:286:GLU:HG3	2.44	0.53
4:A:45:TRP:O	4:A:49:LYS:HG2	2.09	0.53
4:C:185:GLN:OE1	4:D:62:SER:CB	2.53	0.53
4:C:211:TRP:CZ3	4:C:215:VAL:HG11	2.43	0.53
8:X:367:ARG:HE	8:Z:510:VAL:HG22	1.73	0.53
3:7:167:A:OP1	7:S:17:ARG:NH2	2.43	0.52
8:X:427:GLN:C	8:X:429:LEU:H	2.16	0.52
8:X:428:ASN:HD22	8:X:501:ILE:HD12	1.74	0.52
1:1:42:DC:C4'	4:L:119:LYS:HD3	2.26	0.52
1:1:45:DT:H1'	6:Q:59:ASN:ND2	2.23	0.52
6:Q:13:LEU:CD1	6:Q:74:VAL:O	2.57	0.52
1:1:-9:DC:H2''	1:1:-8:DA:C8	2.43	0.52
1:1:7:DA:H2	8:W:290:LYS:HG3	1.75	0.52
1:1:55:DC:OP1	5:O:589:SER:C	2.53	0.52
4:F:67:THR:HG1	13:F:301:MG:MG	1.16	0.52
5:O:478:LYS:HD3	5:O:485:TYR:CE2	2.45	0.52
3:7:169:G:C5'	6:Q:128:LYS:HD3	2.38	0.52
4:C:242:GLY:HA2	14:C:302:ATP:H4'	1.91	0.52
8:Y:523:ARG:HG3	8:Y:526:ARG:CD	2.38	0.52
1:1:63:DC:H5'	5:O:425:THR:OG1	2.09	0.52
2:3:-1:DT:O3'	5:O:418:LEU:HD12	2.04	0.52
5:O:13:PHE:CD1	5:O:15:SER:HB2	2.39	0.52
8:x:576:GLU:CA	8:x:579:ARG:NH2	2.73	0.52
1:1:35:DT:H1'	1:1:36:DG:C5'	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:48:DT:C1'	5:O:270:ASP:OD1	2.58	0.52
2:3:38:DA:P	4:C:121:THR:HG1	2.33	0.52
4:A:157:VAL:O	4:A:158:ARG:C	2.52	0.52
8:X:109:GLU:O	8:X:110:PHE:C	2.51	0.52
8:X:153:TYR:OH	11:5:7:DG:OP2	2.22	0.52
4:I:207:THR:HG22	4:I:211:TRP:CD1	2.44	0.52
4:K:124:ASP:O	4:K:125:PHE:C	2.51	0.52
3:7:234:A:H5''	5:O:240:ARG:NH2	2.25	0.52
4:C:191:ARG:O	4:C:192:ALA:C	2.49	0.52
4:K:54:LYS:HG3	4:L:250:GLU:HG2	1.91	0.52
8:X:355:ARG:NE	8:Z:522:SER:HA	2.12	0.52
8:X:425:GLN:HB2	12:6:12:DC:P	2.50	0.52
3:7:242:U:H5'	5:O:503:HIS:CD2	2.45	0.51
4:B:184:GLU:HG2	4:C:62:SER:OG	2.10	0.51
4:I:260:LEU:CD1	4:I:264:ASP:OD2	2.58	0.51
2:3:-7:DA:H2'	2:3:-6:DC:C6	2.45	0.51
4:C:211:TRP:NE1	4:C:244:LEU:HD23	2.24	0.51
4:E:207:THR:O	4:E:211:TRP:CD1	2.63	0.51
5:O:39:LEU:HD22	5:O:236:MET:HB3	1.92	0.51
4:C:211:TRP:HE3	4:C:215:VAL:CB	2.23	0.51
4:H:85:ARG:HG3	4:H:86:PRO:HD3	1.91	0.51
4:I:207:THR:C	4:I:211:TRP:HD1	2.18	0.51
8:W:180:GLY:C	8:W:181:THR:HG1	2.14	0.51
3:7:47:G:O2'	3:7:143:G:OP1	2.22	0.51
8:x:576:GLU:CA	8:x:579:ARG:HH21	2.23	0.51
3:7:20:U:O4	3:7:21:C:N4	2.44	0.51
4:F:128:ARG:HH11	4:L:181:LYS:HZ2	1.58	0.51
4:L:116:ARG:HH11	6:Q:147:GLU:HG2	1.75	0.51
5:O:17:ARG:NH1	5:O:371:LEU:CB	2.64	0.51
8:W:307:VAL:HG13	8:W:309:HIS:NE2	2.26	0.51
4:I:185:GLN:OE1	4:J:173:THR:CG2	2.43	0.51
4:K:122:VAL:O	4:K:125:PHE:N	2.44	0.51
4:I:191:ARG:NH2	4:J:243:ARG:HH21	1.79	0.51
4:J:53:ARG:NE	4:K:29:LYS:HZ1	2.09	0.51
11:5:9:DG:H2''	11:5:10:DA:C8	2.46	0.51
1:1:1:DT:H5'	8:X:208:ARG:HG2	1.93	0.51
4:C:87:PRO:O	4:C:136:CYS:SG	2.62	0.51
5:O:414:THR:HG22	5:O:414:THR:O	2.11	0.51
8:Z:322:ARG:N	8:Z:323:PRO:HD3	2.25	0.51
3:7:21:C:OP1	4:I:81:GLN:O	2.29	0.50
4:H:187:LEU:HD23	4:H:187:LEU:C	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:13:LEU:HD11	6:Q:75:GLU:HB2	1.94	0.50
8:Z:299:GLN:O	8:Z:302:ALA:N	2.44	0.50
2:3:17:DG:C5	5:O:567:PHE:CZ	2.99	0.50
14:D:302:ATP:H5'1	14:D:302:ATP:C8	2.46	0.50
4:E:187:LEU:HD23	4:E:187:LEU:C	2.36	0.50
8:X:293:ARG:NH2	12:6:19:DT:H4'	2.27	0.50
4:A:187:LEU:C	4:A:187:LEU:HD23	2.37	0.50
4:K:189:ARG:HH22	14:L:302:ATP:PG	2.34	0.50
4:L:31:LYS:HG2	4:L:249:ARG:HH12	1.76	0.50
5:O:325:PHE:HA	5:O:328:PHE:CD2	2.46	0.50
10:4:-19:DT:H2''	10:4:-18:DA:C8	2.45	0.50
4:D:210:MET:CE	8:y:570:ILE:HD11	2.41	0.50
4:F:187:LEU:C	4:F:187:LEU:HD23	2.36	0.50
4:K:112:TYR:HH	6:Q:5:PRO:HG3	1.75	0.50
8:W:58:ARG:HA	8:W:61:TYR:CD2	2.44	0.50
8:Z:519:THR:O	8:Z:522:SER:HB2	2.12	0.50
4:H:47:ASP:OD2	4:H:51:LYS:NZ	2.44	0.50
6:Q:121:LYS:NZ	6:Q:123:ASP:OD1	2.45	0.50
7:S:50:HIS:ND1	7:S:53:ARG:NH2	2.53	0.50
8:X:106:ARG:HH12	10:4:-13:DT:C4'	2.17	0.50
5:O:481:LEU:HD13	5:O:484:ASN:HB2	1.94	0.50
7:S:45:GLU:HG2	7:S:46:HIS:CD2	2.45	0.50
8:X:161:ALA:HB3	8:X:162:PRO:HD3	1.94	0.50
8:X:174:ARG:NH2	9:2:4:DA:N6	2.60	0.50
8:Z:258:HIS:O	8:Z:259:ALA:C	2.53	0.50
1:1:53:DG:OP1	5:O:517:SER:CB	2.60	0.50
3:7:166:G:H4'	7:S:20:ASN:O	2.11	0.50
4:I:144:ASP:OD2	4:I:145:GLU:N	2.43	0.50
1:1:31:DA:N3	1:1:32:DA:C5	2.80	0.50
4:A:159:ASP:C	4:A:161:ALA:H	2.19	0.50
4:B:126:ARG:NH1	4:C:97:HIS:HB3	2.27	0.50
4:F:211:TRP:HZ2	4:F:241:ILE:CD1	2.16	0.50
4:J:192:ALA:HB2	4:K:275:TYR:CZ	2.47	0.50
4:K:122:VAL:O	4:K:123:SER:C	2.53	0.50
8:W:322:ARG:NH1	11:5:4:DA:C2	2.78	0.50
2:3:-7:DA:H2''	2:3:-6:DC:O5'	2.12	0.50
1:1:30:DC:C2'	1:1:31:DA:C8	2.92	0.49
4:H:185:GLN:OE1	4:I:62:SER:CB	2.41	0.49
4:J:93:TYR:HD2	4:J:142:ILE:HB	1.76	0.49
8:Y:416:ARG:CZ	10:4:-7:DC:H5''	2.42	0.49
2:3:17:DG:C4	5:O:567:PHE:CE2	2.98	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Y:527:GLN:O	8:Y:528:LYS:C	2.54	0.49
2:3:53:DT:O2	8:W:290:LYS:CE	2.60	0.49
5:O:279:LEU:HD11	5:O:358:GLU:HG3	1.94	0.49
4:J:93:TYR:OH	4:J:144:ASP:HB2	2.12	0.49
4:J:185:GLN:HE21	4:J:185:GLN:HA	1.76	0.49
5:O:284:VAL:HG22	5:O:353:HIS:CD2	2.47	0.49
8:X:178:TRP:CE3	9:2:1:DT:N3	2.79	0.49
10:4:8:DA:H2'	10:4:9:DC:C6	2.48	0.49
2:3:-1:DT:C1'	5:O:418:LEU:HD12	2.39	0.49
3:7:240:U:O2'	3:7:241:U:H6	1.96	0.49
4:K:105:LEU:HD22	4:K:153:THR:CG2	2.43	0.49
4:L:152:GLU:OE1	4:L:152:GLU:N	2.33	0.49
8:X:106:ARG:HH11	10:4:-13:DT:C4'	2.23	0.49
8:X:293:ARG:NH2	12:6:19:DT:C5'	2.72	0.49
9:2:9:DG:H2''	9:2:10:DA:H8	1.78	0.49
11:5:8:DT:H2''	11:5:9:DG:C8	2.47	0.49
1:1:48:DT:H2'	1:1:49:DA:H8	1.75	0.49
4:C:211:TRP:NE1	4:C:244:LEU:CD2	2.75	0.49
5:O:284:VAL:HG22	5:O:353:HIS:HD2	1.78	0.49
8:X:301:GLY:HA2	8:X:306:PHE:CE2	2.47	0.49
1:1:31:DA:H2''	1:1:32:DA:C8	2.48	0.49
1:1:57:DT:H2'	1:1:58:DC:C6	2.48	0.49
4:B:158:ARG:HD2	4:B:189:ARG:CD	2.43	0.49
4:H:65:GLY:HA2	14:H:302:ATP:PA	2.51	0.49
5:O:418:LEU:C	5:O:418:LEU:HD23	2.38	0.49
2:3:-5:DT:OP2	5:O:309:SER:CB	2.59	0.49
7:S:50:HIS:CE1	7:S:53:ARG:HH21	2.31	0.49
4:F:128:ARG:CD	4:L:181:LYS:HZ2	2.25	0.49
8:W:178:TRP:CD1	11:5:3:DT:P	3.04	0.49
8:W:322:ARG:NH2	11:5:5:DC:O4'	2.46	0.49
8:W:386:ARG:NH2	11:5:5:DC:OP1	2.44	0.49
8:X:58:ARG:HG3	10:4:-26:DA:C5'	2.42	0.49
4:F:128:ARG:HD3	4:L:181:LYS:HZ2	1.76	0.48
4:K:116:ARG:HB3	6:Q:11:LEU:CD2	2.43	0.48
6:Q:20:GLU:OE1	6:Q:28:ARG:NH1	2.46	0.48
8:Y:247:PRO:HA	8:Y:251:VAL:CG2	2.42	0.48
2:3:53:DT:O2	8:W:290:LYS:HE3	2.13	0.48
5:O:31:LEU:HD22	5:O:281:PHE:CD1	2.47	0.48
8:X:58:ARG:HG2	10:4:-26:DA:H5'	1.93	0.48
2:3:27:DT:H2''	2:3:28:DT:H71	1.94	0.48
4:A:85:ARG:HD3	4:H:273:LYS:HD3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:185:GLN:OE1	4:G:62:SER:HB3	2.14	0.48
8:W:306:PHE:CD1	8:W:306:PHE:C	2.91	0.48
1:I:36:DG:H3'	4:I:119:LYS:CD	2.41	0.48
4:H:34:VAL:N	14:H:302:ATP:N1	2.57	0.48
8:X:425:GLN:HB2	12:6:11:DG:O3'	2.13	0.48
3:7:27:G:O6	3:7:31:G:N1	2.47	0.48
3:7:172:C:H2'	3:7:174:G:C8	2.48	0.48
4:C:211:TRP:CE3	4:C:215:VAL:CB	2.96	0.48
4:D:211:TRP:CE3	4:D:215:VAL:HG11	2.49	0.48
4:I:211:TRP:CZ3	4:I:245:ASP:OD1	2.67	0.48
4:L:47:ASP:OD2	4:L:51:LYS:NZ	2.45	0.48
6:Q:95:GLU:HB3	6:Q:96:PRO:CD	2.42	0.48
8:Y:282:GLU:C	8:Y:283:HIS:CD2	2.91	0.48
3:7:242:U:H5'	5:O:503:HIS:HD2	1.77	0.48
4:A:49:LYS:C	4:A:51:LYS:N	2.72	0.48
4:J:93:TYR:CZ	4:J:144:ASP:HB2	2.48	0.48
4:H:185:GLN:HE21	4:H:189:ARG:NH1	2.08	0.48
8:Y:282:GLU:C	8:Y:283:HIS:HD2	2.22	0.48
1:I:2:DA:C2	8:X:343:VAL:HG21	2.48	0.48
1:I:50:DA:H5''	5:O:275:ARG:CG	2.31	0.48
4:I:121:THR:HG22	4:I:124:ASP:CG	2.37	0.48
6:Q:149:GLY:CA	6:Q:158:PHE:CD1	2.95	0.48
8:Y:518:ALA:O	8:Y:519:THR:HB	2.14	0.48
8:W:88:GLN:O	8:W:88:GLN:HG3	2.14	0.48
9:2:16:DT:H2''	9:2:17:DA:N7	2.29	0.48
10:4:-9:DC:H2''	10:4:-8:DA:C8	2.49	0.48
4:B:65:GLY:HA2	14:B:302:ATP:O2A	2.14	0.48
4:D:152:GLU:OE1	4:D:152:GLU:N	2.33	0.48
4:E:211:TRP:CZ2	4:E:241:ILE:CD1	2.83	0.48
4:F:211:TRP:NE1	4:F:244:LEU:HD23	2.27	0.48
4:H:264:ASP:OD2	4:H:267:VAL:CG1	2.48	0.48
8:W:346:ARG:HD2	10:4:2:DT:H72	1.95	0.48
4:A:141:LEU:HG	4:A:168:VAL:HG22	1.96	0.47
4:C:202:GLU:OE2	8:X:476:GLY:HA2	2.13	0.47
4:I:260:LEU:HD11	4:I:264:ASP:OD2	2.14	0.47
8:X:426:PHE:CD1	8:X:427:GLN:HG2	2.49	0.47
3:7:168:U:OP1	7:S:73:LYS:NZ	2.47	0.47
3:7:240:U:O2'	3:7:241:U:H5'	2.14	0.47
4:A:134:LYS:HE3	4:A:164:LEU:CD2	2.44	0.47
4:K:185:GLN:HE22	4:L:62:SER:CB	2.17	0.47
8:W:178:TRP:CD2	11:5:1:DT:H73	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:360:GLU:OE2	8:Y:521:LYS:CE	2.61	0.47
8:X:426:PHE:CE1	8:X:427:GLN:HG2	2.48	0.47
3:7:51:A:O2'	3:7:52:A:H5'	2.14	0.47
3:7:115:G:O2'	3:7:154:A:N1	2.40	0.47
4:J:222:SER:HB3	4:J:224:LEU:CD1	2.43	0.47
8:W:178:TRP:HD1	11:5:3:DT:OP2	1.97	0.47
1:1:35:DT:C2	1:1:36:DG:C5	3.02	0.47
1:1:36:DG:C2	1:1:37:DA:C4	3.03	0.47
8:W:178:TRP:CE3	11:5:1:DT:C5	3.02	0.47
2:3:-2:DT:O3'	5:O:414:THR:CG2	2.47	0.47
4:C:152:GLU:OE1	4:C:152:GLU:N	2.33	0.47
4:I:254:ARG:CD	4:I:267:VAL:CG1	2.79	0.47
11:5:12:DT:H2''	11:5:13:DA:C8	2.50	0.47
1:1:1:DT:H5'	8:X:208:ARG:CG	2.45	0.47
1:1:68:DC:H2''	1:1:69:DA:C8	2.49	0.47
4:A:93:TYR:CD1	4:A:142:ILE:HG22	2.49	0.47
4:C:53:ARG:HA	4:C:53:ARG:HD3	1.57	0.47
5:O:9:ARG:NH2	5:O:370:HIS:HD2	2.09	0.47
5:O:412:SER:CB	5:O:415:GLN:HB2	2.44	0.47
4:A:92:VAL:HB	4:A:141:LEU:HA	1.96	0.47
5:O:42:HIS:CE1	5:O:44:ASP:CA	2.97	0.47
8:X:152:ASN:ND2	10:4:-10:DT:OP2	2.47	0.47
1:1:8:DT:H1'	8:W:290:LYS:HD2	1.97	0.47
2:3:29:DT:C2	2:3:30:DG:C8	3.03	0.47
4:A:65:GLY:HA2	14:A:302:ATP:O2A	2.15	0.47
8:Z:463:ASN:H	8:Z:463:ASN:ND2	2.13	0.47
4:E:178:ALA:HB2	8:W:438:GLY:C	2.40	0.47
4:E:207:THR:HG22	4:E:211:TRP:CD1	2.50	0.47
4:F:152:GLU:OE1	4:F:152:GLU:N	2.33	0.47
8:X:495:ARG:CZ	12:6:13:DT:H5'	2.44	0.47
2:3:55:DT:H5'	8:W:289:GLY:HA2	1.97	0.46
4:E:207:THR:CG2	4:E:211:TRP:HE1	2.25	0.46
5:O:595:GLN:HA	5:O:598:GLN:OE1	2.15	0.46
8:W:178:TRP:CD2	11:5:1:DT:C7	2.79	0.46
1:1:24:DT:H2'	1:1:25:DA:C8	2.50	0.46
1:1:34:DT:H2''	1:1:35:DT:OP2	2.15	0.46
1:1:42:DC:H4'	4:L:119:LYS:HZ3	1.79	0.46
4:A:141:LEU:CD1	4:A:141:LEU:O	2.54	0.46
4:D:99:LYS:C	4:D:150:LYS:HE2	2.40	0.46
9:2:8:DT:H2''	9:2:9:DG:C8	2.50	0.46
9:2:19:DC:C6	9:2:20:DT:H72	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2:DA:C6	8:X:343:VAL:HG21	2.50	0.46
1:1:62:DA:N7	5:O:287:THR:HG23	2.31	0.46
1:1:64:DC:OP2	5:O:428:ARG:NH2	2.48	0.46
4:A:93:TYR:CZ	4:A:144:ASP:HB2	2.50	0.46
4:D:62:SER:O	14:D:302:ATP:O3B	2.33	0.46
4:I:185:GLN:NE2	4:J:62:SER:HB2	2.29	0.46
5:O:292:VAL:HG12	5:O:304:HIS:NE2	2.24	0.46
4:C:213:GLN:O	4:C:213:GLN:HG2	2.15	0.46
4:F:218:LEU:HD11	4:F:252:ALA:CB	2.45	0.46
2:3:-2:DT:H2''	2:3:-1:DT:C6	2.50	0.46
10:4:-13:DT:H2''	10:4:-12:DA:C8	2.51	0.46
11:5:5:DC:H2''	11:5:6:DA:C8	2.50	0.46
3:7:242:U:H2'	3:7:243:A:C8	2.50	0.46
4:F:66:LYS:NZ	14:F:302:ATP:O2G	2.48	0.46
11:5:18:DT:H2''	11:5:19:DA:C8	2.50	0.46
6:Q:94:HIS:ND1	6:Q:94:HIS:C	2.72	0.46
3:7:41:A:OP1	5:O:478:LYS:CE	2.63	0.46
8:W:258:HIS:CD2	8:W:263:LYS:HE3	2.50	0.46
8:W:360:GLU:CD	8:Y:521:LYS:CE	2.89	0.46
8:X:289:GLY:CA	12:6:20:DC:H5'	2.46	0.46
8:W:306:PHE:O	8:W:306:PHE:HD1	1.87	0.46
8:W:360:GLU:OE2	8:Y:521:LYS:NZ	2.48	0.46
11:5:9:DG:H2''	11:5:10:DA:H8	1.80	0.46
11:5:25:DT:H2'	11:5:26:DT:H71	1.96	0.46
1:1:27:DA:H2'	1:1:28:DT:H71	1.98	0.45
1:1:48:DT:O4'	5:O:266:LYS:NZ	2.49	0.45
4:C:193:HIS:CG	4:C:193:HIS:O	2.66	0.45
4:F:211:TRP:HE3	4:F:215:VAL:CG2	2.30	0.45
4:K:185:GLN:NE2	14:L:302:ATP:O1G	2.47	0.45
8:Y:523:ARG:CD	8:Y:526:ARG:HE	2.28	0.45
1:1:50:DA:H4'	5:O:275:ARG:CG	2.46	0.45
3:7:239:A:H5'	5:O:586:HIS:CE1	2.52	0.45
4:A:140:MET:HA	4:A:167:ALA:O	2.16	0.45
4:I:191:ARG:NE	4:J:243:ARG:CZ	2.72	0.45
8:X:495:ARG:CZ	12:6:13:DT:C5'	2.94	0.45
1:1:38:DG:C8	1:1:39:DT:H72	2.51	0.45
1:1:62:DA:N7	5:O:287:THR:OG1	2.47	0.45
4:L:115:TYR:OH	6:Q:155:ARG:HG2	2.16	0.45
6:Q:149:GLY:CA	6:Q:158:PHE:HD1	2.26	0.45
11:5:20:DT:H2''	11:5:21:DG:H5''	1.98	0.45
4:A:159:ASP:O	4:A:160:ILE:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:97:HIS:C	4:J:148:ARG:HD3	2.42	0.45
4:J:222:SER:O	4:J:223:ASN:C	2.59	0.45
1:1:56:DT:H2'	1:1:57:DT:C6	2.51	0.45
3:7:25:C:H42	3:7:34:G:H1	1.63	0.45
3:7:106:G:H4'	7:S:55:GLY:HA3	1.99	0.45
4:C:180:ILE:HG22	4:C:187:LEU:HD13	1.99	0.45
8:x:576:GLU:HA	8:x:579:ARG:HH21	1.80	0.45
1:1:48:DT:C2'	5:O:270:ASP:OD1	2.65	0.45
2:3:47:DC:OP2	8:W:416:ARG:NH1	2.50	0.45
4:B:185:GLN:CD	4:C:173:THR:CG2	2.84	0.45
4:I:65:GLY:HA2	14:I:302:ATP:PA	2.56	0.45
8:Y:416:ARG:NE	10:4:-7:DC:H5''	2.32	0.45
3:7:85:U:O2'	5:O:318:GLY:C	2.60	0.45
3:7:239:A:C4'	5:O:586:HIS:CD2	3.00	0.45
4:A:116:ARG:NH2	4:G:61:GLU:HB3	2.31	0.45
4:D:35:PRO:HD3	8:y:571:GLU:O	2.16	0.45
4:D:110:THR:HG21	4:D:117:VAL:HG22	1.98	0.45
8:X:147:ASP:OD1	8:X:148:SER:N	2.49	0.45
2:3:48:DA:OP1	8:W:495:ARG:CZ	2.64	0.45
8:W:177:GLY:O	11:5:1:DT:C6	2.70	0.45
1:1:16:DC:H2''	1:1:17:DA:H8	1.82	0.45
4:A:81:GLN:HE22	4:A:87:PRO:HB3	1.81	0.45
4:D:211:TRP:CZ3	4:D:215:VAL:HG11	2.52	0.45
5:O:357:LEU:HD21	5:O:374:TYR:OH	2.16	0.45
8:X:289:GLY:N	12:6:20:DC:H5'	2.32	0.45
8:Z:519:THR:HA	8:Z:522:SER:CB	2.46	0.45
4:B:126:ARG:CZ	4:C:97:HIS:ND1	2.80	0.45
4:K:47:ASP:OD2	4:K:51:LYS:HE3	2.17	0.45
8:W:343:VAL:HG23	10:4:2:DT:C5	2.51	0.45
8:X:495:ARG:NE	12:6:13:DT:C5'	2.72	0.45
11:5:16:DT:H2''	11:5:17:DA:N7	2.31	0.45
1:1:36:DG:C4	1:1:37:DA:C8	3.05	0.44
1:1:57:DT:H2'	1:1:58:DC:H6	1.82	0.44
3:7:239:A:C5'	5:O:586:HIS:NE2	2.76	0.44
4:L:115:TYR:OH	6:Q:155:ARG:CG	2.65	0.44
8:Z:452:ASP:OD1	8:Z:452:ASP:C	2.59	0.44
1:1:49:DA:C2'	1:1:50:DA:H5'	2.46	0.44
2:3:25:DA:H5''	4:J:122:VAL:CG2	2.47	0.44
3:7:17:A:H61	3:7:44:U:H3	1.65	0.44
4:A:93:TYR:CD1	4:A:142:ILE:HB	2.47	0.44
14:F:302:ATP:H5'1	14:F:302:ATP:H8	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:2:5:DC:H2''	9:2:6:DA:C8	2.52	0.44
3:7:15:G:N3	3:7:51:A:H2	2.15	0.44
4:A:62:SER:HB2	14:A:302:ATP:O3G	2.16	0.44
4:H:185:GLN:NE2	4:I:62:SER:HB3	2.13	0.44
4:J:185:GLN:HE21	4:J:189:ARG:HH12	1.64	0.44
5:O:42:HIS:CE1	5:O:44:ASP:H	2.36	0.44
3:7:203:C:N3	5:O:17:ARG:NE	2.66	0.44
4:D:65:GLY:HA2	14:D:302:ATP:PA	2.58	0.44
4:L:97:HIS:HA	4:L:148:ARG:HH11	1.83	0.44
1:1:32:DA:H2''	1:1:33:DA:O5'	2.16	0.44
5:O:35:LEU:C	5:O:39:LEU:HG	2.41	0.44
8:Y:247:PRO:HA	8:Y:251:VAL:CG1	2.48	0.44
1:1:-23:DG:H2''	1:1:-22:DA:C8	2.52	0.44
3:7:55:A:C2	5:O:497:TYR:CB	2.93	0.44
3:7:239:A:H4'	5:O:586:HIS:CD2	2.52	0.44
8:X:99:ARG:NH1	10:4:-15:DA:N3	2.65	0.44
14:B:302:ATP:H8	14:B:302:ATP:C5'	2.17	0.44
4:J:38:GLN:HG3	4:J:196:PHE:CE2	2.52	0.44
5:O:463:VAL:CG2	5:O:534:LEU:HD21	2.48	0.44
8:X:58:ARG:HG3	10:4:-26:DA:H5'	1.98	0.44
3:7:80:A:H2'	3:7:81:G:C8	2.53	0.44
4:A:32:SER:O	14:A:302:ATP:H2	2.01	0.44
4:B:189:ARG:NH2	14:C:302:ATP:O1G	2.51	0.44
8:W:177:GLY:O	11:5:1:DT:H6	2.00	0.44
8:Z:481:GLN:OE1	8:Z:481:GLN:N	2.46	0.44
4:B:40:LYS:NZ	4:B:44:ASP:OD2	2.50	0.44
4:F:134:LYS:HE2	4:F:164:LEU:CD2	2.47	0.44
4:J:185:GLN:HE21	4:J:189:ARG:NH1	2.16	0.44
8:X:356:LEU:HD23	8:Z:521:LYS:HG3	1.98	0.44
1:1:17:DA:H2'	1:1:18:DT:C6	2.53	0.43
1:1:50:DA:O5'	1:1:50:DA:H8	2.00	0.43
2:3:-7:DA:H4'	2:3:-6:DC:OP1	2.18	0.43
2:3:28:DT:C6	2:3:29:DT:H73	2.53	0.43
4:E:211:TRP:NE1	4:E:244:LEU:HD23	2.33	0.43
8:W:353:ASP:CA	8:Y:524:LYS:HD2	2.47	0.43
10:4:7:DT:H2'	10:4:8:DA:H8	1.82	0.43
1:1:-24:DC:H5	8:W:77:ARG:HH12	1.22	0.43
3:7:87:C:O2	5:O:321:GLN:OE1	2.35	0.43
4:D:35:PRO:HG2	8:y:570:ILE:HD12	2.00	0.43
4:I:185:GLN:CD	4:J:62:SER:HB3	2.43	0.43
1:1:64:DC:H2''	1:1:65:DA:H8	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:180:ILE:C	4:C:182:ARG:H	2.26	0.43
4:K:122:VAL:HG13	4:K:123:SER:N	2.33	0.43
8:Y:454:THR:HG23	8:Y:482:LEU:H	1.83	0.43
9:2:7:DG:H2'	9:2:8:DT:H71	1.99	0.43
1:1:13:DG:H5''	4:B:182:ARG:HH22	1.84	0.43
1:1:17:DA:H2''	1:1:18:DT:O5'	2.17	0.43
2:3:-1:DT:P	5:O:414:THR:CB	3.06	0.43
4:A:159:ASP:O	4:A:161:ALA:N	2.51	0.43
4:C:57:ARG:NH1	4:C:191:ARG:O	2.51	0.43
4:K:20:TRP:CE3	4:K:21:LEU:CD2	2.91	0.43
4:L:114:LYS:HG2	4:L:116:ARG:NH2	2.33	0.43
3:7:50:A:O5'	3:7:50:A:H8	2.01	0.43
3:7:203:C:N3	5:O:17:ARG:CD	2.82	0.43
3:7:239:A:H5'	5:O:586:HIS:HE2	1.82	0.43
4:F:134:LYS:CE	4:F:164:LEU:CD2	2.96	0.43
1:1:-4:DT:H2''	1:1:-3:DA:C8	2.54	0.43
4:A:40:LYS:NZ	4:A:44:ASP:OD2	2.50	0.43
4:K:116:ARG:HB3	6:Q:11:LEU:HD21	1.99	0.43
4:L:65:GLY:HA2	14:L:302:ATP:PA	2.59	0.43
5:O:446:HIS:ND1	5:O:447:ILE:HG13	2.34	0.43
4:E:185:GLN:OE1	4:F:62:SER:CB	2.67	0.43
8:Y:434:GLU:OE2	8:Y:473:HIS:CE1	2.71	0.43
3:7:16:C:H1'	3:7:50:A:H2	1.83	0.43
3:7:49:U:O2'	3:7:50:A:OP1	2.33	0.43
4:D:35:PRO:HG3	8:y:571:GLU:O	2.19	0.43
4:F:26:ALA:HA	4:F:29:LYS:HE3	2.01	0.43
4:I:265:LYS:O	4:I:269:GLN:HG3	2.19	0.43
1:1:-16:DA:H2''	1:1:-15:DA:C8	2.53	0.43
4:B:184:GLU:OE2	4:C:61:GLU:HB3	2.18	0.43
4:G:188:GLU:HG3	4:H:62:SER:OG	2.19	0.43
5:O:12:SER:OG	5:O:16:ASN:HB2	2.18	0.43
8:Y:518:ALA:O	8:Y:520:LYS:N	2.49	0.43
9:2:20:DT:H2''	9:2:21:DG:H5''	2.01	0.43
12:6:10:DC:H2''	12:6:11:DG:C8	2.53	0.43
3:7:41:A:P	5:O:478:LYS:CE	2.99	0.43
3:7:99:G:H2'	3:7:100:G:H8	1.84	0.43
3:7:101:U:O2'	3:7:102:A:H8	2.02	0.43
4:C:116:ARG:CZ	4:H:184:GLU:OE1	2.67	0.43
4:L:115:TYR:O	4:L:116:ARG:C	2.62	0.43
8:W:81:ARG:NH1	9:2:20:DT:H71	2.28	0.43
8:Y:452:ASP:C	8:Y:452:ASP:OD1	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:28:DT:H2''	1:1:29:DG:H8	1.83	0.42
3:7:32:C:H2'	3:7:33:A:C8	2.54	0.42
3:7:85:U:O2'	5:O:317:CYS:O	2.25	0.42
4:K:112:TYR:OH	6:Q:5:PRO:CG	2.64	0.42
1:1:31:DA:H2''	1:1:32:DA:H8	1.84	0.42
3:7:244:A:H5'	7:S:54:ARG:HG3	2.00	0.42
4:G:99:LYS:C	4:G:150:LYS:HE3	2.44	0.42
4:J:192:ALA:HB2	4:K:275:TYR:CE2	2.54	0.42
4:L:116:ARG:NH1	6:Q:148:ASP:OD1	2.52	0.42
9:2:16:DT:H2''	9:2:17:DA:C8	2.54	0.42
4:F:187:LEU:HD23	4:F:187:LEU:O	2.20	0.42
4:K:191:ARG:CD	4:L:243:ARG:NE	2.79	0.42
8:X:289:GLY:HA2	12:6:20:DC:H5'	2.01	0.42
3:7:6:A:N3	3:7:150:C:O2'	2.42	0.42
4:A:128:ARG:HD2	4:A:132:VAL:HG13	2.02	0.42
4:E:187:LEU:HD23	4:E:187:LEU:O	2.19	0.42
4:F:218:LEU:CD2	4:F:256:LEU:CD2	2.68	0.42
8:X:427:GLN:O	8:X:429:LEU:N	2.52	0.42
8:X:504:GLN:N	8:X:504:GLN:OE1	2.53	0.42
9:2:2:DG:H2'	9:2:3:DT:H71	2.00	0.42
10:4:-4:DT:H2''	10:4:-3:DA:C8	2.54	0.42
4:A:82:GLU:CD	4:H:273:LYS:NZ	2.77	0.42
4:G:228:GLU:HG2	4:G:231:ARG:NH2	2.34	0.42
4:J:185:GLN:NE2	4:K:62:SER:HB2	2.34	0.42
8:Y:448:PHE:CD2	8:Y:448:PHE:C	2.97	0.42
10:4:-23:DG:H2''	10:4:-22:DA:C8	2.54	0.42
1:1:31:DA:H2'	1:1:31:DA:OP2	2.20	0.42
3:7:50:A:H8	3:7:50:A:C5'	2.33	0.42
3:7:242:U:H2'	3:7:243:A:H8	1.83	0.42
4:J:193:HIS:CE1	4:K:274:GLU:O	2.73	0.42
4:K:117:VAL:HG11	6:Q:35:LEU:HD21	2.01	0.42
5:O:412:SER:CB	5:O:415:GLN:CB	2.98	0.42
8:X:428:ASN:OD1	12:6:13:DT:OP2	2.38	0.42
9:2:21:DG:C8	9:2:22:DT:H72	2.54	0.42
3:7:241:U:P	5:O:579:LYS:HZ2	2.42	0.42
4:A:49:LYS:O	4:A:51:LYS:N	2.51	0.42
4:C:211:TRP:HZ3	4:C:215:VAL:CG2	2.18	0.42
4:H:184:GLU:OE2	4:I:61:GLU:CD	2.59	0.42
5:O:478:LYS:HD3	5:O:485:TYR:HE2	1.82	0.42
2:3:45:DC:H2''	2:3:46:DG:C8	2.55	0.42
8:W:57:ASP:O	8:W:61:TYR:CD2	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:32:DA:C5	1:1:33:DA:C5	3.07	0.42
4:A:187:LEU:HD23	4:A:187:LEU:O	2.20	0.42
4:F:228:GLU:H	4:F:228:GLU:CD	2.12	0.42
8:W:343:VAL:HG21	10:4:2:DT:N3	2.35	0.42
3:7:167:A:H5''	7:S:17:ARG:HH22	1.82	0.42
4:A:159:ASP:O	4:A:162:GLU:N	2.53	0.42
4:G:158:ARG:HD3	4:G:189:ARG:HH11	1.56	0.42
8:X:428:ASN:ND2	12:6:13:DT:OP1	2.44	0.42
8:Z:323:PRO:O	8:Z:327:LEU:HG	2.20	0.42
10:4:-24:DC:H2''	10:4:-23:DG:H8	1.84	0.42
1:1:-13:DT:C6	1:1:-12:DT:H72	2.55	0.41
1:1:61:DA:H2''	1:1:62:DA:C8	2.55	0.41
3:7:48:U:H5	3:7:50:A:C5	2.37	0.41
4:F:99:LYS:C	4:F:150:LYS:HE3	2.44	0.41
4:H:187:LEU:HD23	4:H:187:LEU:O	2.20	0.41
4:I:92:VAL:HA	4:I:112:TYR:CE1	2.55	0.41
8:W:174:ARG:NH2	11:5:4:DA:N6	2.68	0.41
4:C:128:ARG:HD3	4:I:181:LYS:HZ2	1.85	0.41
4:I:68:VAL:HG21	14:I:302:ATP:H2'	2.02	0.41
4:J:185:GLN:NE2	4:J:189:ARG:NH1	2.67	0.41
6:Q:99:LEU:HD21	6:Q:158:PHE:HD2	1.84	0.41
8:X:428:ASN:CB	8:X:506:LEU:HD11	2.50	0.41
10:4:-24:DC:H2''	10:4:-23:DG:C8	2.54	0.41
2:3:35:DT:H2''	2:3:36:DA:OP2	2.19	0.41
4:H:99:LYS:C	4:H:150:LYS:HE3	2.43	0.41
8:Y:231:ASP:OD1	8:Y:231:ASP:C	2.64	0.41
1:1:32:DA:C4	1:1:33:DA:N7	2.89	0.41
2:3:28:DT:C5	2:3:29:DT:H73	2.55	0.41
3:7:150:C:H2'	3:7:151:A:H8	1.85	0.41
3:7:167:A:C5'	7:S:17:ARG:NH2	2.83	0.41
4:C:66:LYS:NZ	14:C:302:ATP:O2G	2.52	0.41
4:F:92:VAL:HG13	4:F:112:TYR:CD1	2.55	0.41
4:L:65:GLY:HA2	14:L:302:ATP:O1A	2.20	0.41
8:x:576:GLU:HB2	8:x:579:ARG:NH2	2.21	0.41
1:1:-12:DT:H71	8:W:158:ARG:CZ	2.50	0.41
2:3:31:DC:H2''	2:3:32:DA:C8	2.55	0.41
4:J:93:TYR:HD2	4:J:142:ILE:CG2	2.34	0.41
7:S:50:HIS:CE1	7:S:53:ARG:NH2	2.88	0.41
8:X:131:PRO:HD2	11:5:7:DG:OP1	2.21	0.41
10:4:0:DT:H2'	10:4:1:DC:C6	2.56	0.41
4:B:126:ARG:HD2	4:C:97:HIS:CE1	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:185:GLN:HE21	4:I:189:ARG:NH1	2.10	0.41
5:O:292:VAL:HB	5:O:304:HIS:CD2	2.48	0.41
5:O:292:VAL:HG11	5:O:304:HIS:CE1	2.54	0.41
9:2:9:DG:H2''	9:2:10:DA:C8	2.55	0.41
4:E:99:LYS:C	4:E:150:LYS:HE3	2.44	0.41
4:H:61:GLU:O	4:H:66:LYS:NZ	2.54	0.41
5:O:17:ARG:HH11	5:O:371:LEU:HD12	1.75	0.41
1:1:-24:DC:N1	8:W:77:ARG:NH2	2.47	0.41
1:1:37:DA:H2''	1:1:38:DG:O5'	2.21	0.41
3:7:239:A:OP1	5:O:556:GLN:HG2	2.21	0.41
4:B:103:LYS:CG	4:B:122:VAL:HG22	2.50	0.41
4:C:126:ARG:NH1	4:D:97:HIS:CB	2.84	0.41
4:D:211:TRP:CZ3	4:D:245:ASP:OD1	2.74	0.41
4:L:65:GLY:HA2	14:L:302:ATP:O3A	2.20	0.41
11:5:16:DT:H2''	11:5:17:DA:C8	2.56	0.41
1:1:-26:DG:OP2	8:W:66:ARG:NH2	2.54	0.41
2:3:28:DT:C2	2:3:29:DT:C5	3.08	0.41
4:C:126:ARG:NH1	4:D:97:HIS:HB3	2.35	0.41
4:C:126:ARG:CZ	4:D:97:HIS:HB3	2.51	0.41
4:E:152:GLU:OE1	4:E:152:GLU:N	2.33	0.41
4:G:66:LYS:NZ	14:G:302:ATP:O2G	2.39	0.41
4:G:152:GLU:OE1	4:G:152:GLU:N	2.33	0.41
4:I:76:ARG:HB2	4:I:77:HIS:ND1	2.35	0.41
4:I:189:ARG:NH2	14:J:302:ATP:O3G	2.52	0.41
4:J:66:LYS:NZ	14:J:302:ATP:O2G	2.45	0.41
5:O:14:GLU:OE2	5:O:366:TRP:NE1	2.50	0.41
8:X:408:ILE:HD12	8:X:409:CYS:N	2.35	0.41
8:Z:454:THR:HG23	8:Z:482:LEU:H	1.86	0.41
8:X:322:ARG:HD3	9:2:3:DT:O2	2.20	0.41
10:4:-17:DT:H2''	10:4:-16:DA:N7	2.36	0.41
1:1:20:DT:H2''	1:1:21:DA:O5'	2.20	0.40
3:7:185:U:H2'	3:7:186:A:C8	2.56	0.40
8:W:325:LYS:HD2	10:4:-3:DA:N3	2.37	0.40
3:7:51:A:H8	3:7:51:A:O5'	2.04	0.40
4:A:82:GLU:OE1	4:H:273:LYS:NZ	2.55	0.40
4:C:126:ARG:CD	4:D:97:HIS:CE1	3.03	0.40
4:I:211:TRP:HZ3	4:I:245:ASP:OD1	2.03	0.40
8:W:356:LEU:HD23	8:Y:521:LYS:HD3	2.03	0.40
2:3:47:DC:OP1	8:W:425:GLN:HB3	2.22	0.40
3:7:70:G:N1	3:7:79:C:O2	2.53	0.40
4:A:48:GLY:O	4:A:51:LYS:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:93:TYR:CE1	4:A:142:ILE:HG22	2.56	0.40
4:D:99:LYS:CB	4:D:150:LYS:HZ3	2.32	0.40
4:E:211:TRP:CD1	4:E:244:LEU:HD21	2.55	0.40
4:F:185:GLN:OE1	4:G:62:SER:CB	2.69	0.40
4:L:115:TYR:CZ	6:Q:155:ARG:CD	2.94	0.40
8:X:495:ARG:HE	12:6:13:DT:H5'	1.76	0.40
3:7:243:A:O3'	7:S:54:ARG:HD2	2.21	0.40
4:H:27:ARG:HG2	4:H:27:ARG:HH11	1.86	0.40
8:x:576:GLU:HA	8:x:579:ARG:CZ	2.51	0.40
8:X:178:TRP:HB2	8:X:380:ARG:HE	1.86	0.40
4:K:105:LEU:CD2	4:K:153:THR:HG22	2.49	0.40
5:O:42:HIS:CE1	5:O:44:ASP:N	2.90	0.40
8:W:38:LEU:HB2	8:W:43:GLN:NE2	2.37	0.40
8:X:238:MET:HE3	8:X:277:THR:HG22	2.04	0.40
12:6:16:DG:H2'	12:6:17:DT:H71	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	255/276 (92%)	248 (97%)	6 (2%)	1 (0%)	30	60
4	B	255/276 (92%)	254 (100%)	1 (0%)	0	100	100
4	C	255/276 (92%)	247 (97%)	8 (3%)	0	100	100
4	D	255/276 (92%)	248 (97%)	7 (3%)	0	100	100
4	E	255/276 (92%)	252 (99%)	3 (1%)	0	100	100
4	F	255/276 (92%)	250 (98%)	5 (2%)	0	100	100
4	G	255/276 (92%)	250 (98%)	5 (2%)	0	100	100
4	H	255/276 (92%)	252 (99%)	2 (1%)	1 (0%)	30	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	I	255/276 (92%)	254 (100%)	1 (0%)	0	100	100
4	J	255/276 (92%)	250 (98%)	5 (2%)	0	100	100
4	K	255/276 (92%)	250 (98%)	5 (2%)	0	100	100
4	L	255/276 (92%)	249 (98%)	6 (2%)	0	100	100
5	O	595/639 (93%)	580 (98%)	14 (2%)	1 (0%)	43	72
6	Q	162/167 (97%)	151 (93%)	10 (6%)	1 (1%)	21	52
7	S	85/89 (96%)	83 (98%)	1 (1%)	1 (1%)	10	40
8	W	512/584 (88%)	493 (96%)	19 (4%)	0	100	100
8	X	503/584 (86%)	484 (96%)	17 (3%)	2 (0%)	30	60
8	Y	296/584 (51%)	284 (96%)	12 (4%)	0	100	100
8	Z	293/584 (50%)	282 (96%)	9 (3%)	2 (1%)	18	50
8	w	12/584 (2%)	12 (100%)	0	0	100	100
8	x	12/584 (2%)	12 (100%)	0	0	100	100
8	y	12/584 (2%)	12 (100%)	0	0	100	100
8	z	12/584 (2%)	12 (100%)	0	0	100	100
All	All	5554/8879 (63%)	5409 (97%)	136 (2%)	9 (0%)	44	72

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	61	GLU
5	O	413	ASP
8	X	176	PRO
4	A	50	ARG
8	Z	323	PRO
8	Z	464	ASN
6	Q	95	GLU
7	S	23	GLY
8	X	314	PRO

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	224/238 (94%)	221 (99%)	3 (1%)	61	71
4	B	224/238 (94%)	224 (100%)	0	100	100
4	C	224/238 (94%)	221 (99%)	3 (1%)	61	71
4	D	224/238 (94%)	224 (100%)	0	100	100
4	E	224/238 (94%)	224 (100%)	0	100	100
4	F	224/238 (94%)	224 (100%)	0	100	100
4	G	224/238 (94%)	223 (100%)	1 (0%)	84	81
4	H	224/238 (94%)	224 (100%)	0	100	100
4	I	224/238 (94%)	224 (100%)	0	100	100
4	J	224/238 (94%)	223 (100%)	1 (0%)	84	81
4	K	224/238 (94%)	223 (100%)	1 (0%)	84	81
4	L	224/238 (94%)	223 (100%)	1 (0%)	84	81
5	O	529/564 (94%)	529 (100%)	0	100	100
6	Q	136/139 (98%)	136 (100%)	0	100	100
7	S	75/77 (97%)	75 (100%)	0	100	100
8	W	448/512 (88%)	448 (100%)	0	100	100
8	X	442/512 (86%)	440 (100%)	2 (0%)	81	80
8	Y	264/512 (52%)	263 (100%)	1 (0%)	84	81
8	Z	261/512 (51%)	260 (100%)	1 (0%)	84	81
8	w	13/512 (2%)	13 (100%)	0	100	100
8	x	13/512 (2%)	13 (100%)	0	100	100
8	y	13/512 (2%)	13 (100%)	0	100	100
8	z	13/512 (2%)	13 (100%)	0	100	100
All	All	4895/7732 (63%)	4881 (100%)	14 (0%)	84	83

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	50	ARG
4	A	51	LYS
4	A	182	ARG
4	C	53	ARG
4	C	54	LYS

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Mol	Chain	Res	Type
4	C	191	ARG
4	G	185	GLN
4	J	185	GLN
4	K	153	THR
4	L	150	LYS
8	X	355	ARG
8	X	408	ILE
8	Y	251	VAL
8	Z	463	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	81	GLN
4	A	185	GLN
4	E	193	HIS
4	G	185	GLN
4	G	193	HIS
4	H	77	HIS
4	H	185	GLN
4	I	80	GLN
4	I	185	GLN
4	J	80	GLN
4	J	81	GLN
4	J	185	GLN
4	K	185	GLN
4	L	269	GLN
5	O	42	HIS
5	O	49	GLN
5	O	104	GLN
5	O	116	ASN
5	O	353	HIS
5	O	370	HIS
5	O	423	GLN
5	O	500	HIS
5	O	506	GLN
5	O	595	GLN
5	O	620	HIS
6	Q	57	HIS
6	Q	137	GLN
7	S	42	HIS
7	S	46	HIS

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Mol	Chain	Res	Type
8	W	50	GLN
8	W	217	HIS
8	W	299	GLN
8	W	344	GLN
8	W	445	ASN
8	X	43	GLN
8	X	50	GLN
8	X	425	GLN
8	X	427	GLN
8	X	461	GLN
8	X	465	GLN
8	Y	384	GLN
8	Y	473	HIS
8	Y	503	ASN
8	Z	241	ASN
8	Z	296	HIS
8	Z	445	ASN
8	Z	463	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	7	227/265 (85%)	55 (24%)	5 (2%)

All (55) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	7	9	A
3	7	15	G
3	7	18	A
3	7	22	A
3	7	24	G
3	7	26	U
3	7	28	C
3	7	30	U
3	7	31	G
3	7	32	C
3	7	35	C
3	7	40	G
3	7	48	U
3	7	49	U

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Mol	Chain	Res	Type
3	7	50	A
3	7	51	A
3	7	55	A
3	7	56	G
3	7	61	A
3	7	66	G
3	7	80	A
3	7	85	U
3	7	86	G
3	7	99	G
3	7	102	A
3	7	117	U
3	7	118	G
3	7	129	U
3	7	130	A
3	7	131	G
3	7	137	A
3	7	138	U
3	7	139	A
3	7	140	G
3	7	142	U
3	7	147	U
3	7	155	A
3	7	169	G
3	7	170	U
3	7	172	C
3	7	173	U
3	7	174	G
3	7	177	G
3	7	193	C
3	7	200	G
3	7	204	A
3	7	205	A
3	7	226	G
3	7	227	A
3	7	228	A
3	7	231	G
3	7	232	A
3	7	239	A
3	7	241	U
3	7	242	U

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	7	48	U
3	7	49	U
3	7	50	A
3	7	130	A
3	7	173	U

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, 14 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
14	ATP	J	302	13	32,33,33	0.82	0	48,52,52	0.67	0
14	ATP	B	302	13	32,33,33	0.83	0	48,52,52	0.75	0
14	ATP	E	302	13	32,33,33	0.86	0	48,52,52	0.65	0
14	ATP	C	302	13	32,33,33	0.79	0	48,52,52	0.67	0
14	ATP	D	302	13	32,33,33	0.83	0	48,52,52	0.74	0
14	ATP	G	302	13	32,33,33	0.87	0	48,52,52	0.72	0
14	ATP	H	302	13	32,33,33	0.73	0	48,52,52	0.64	0
14	ATP	I	302	13	32,33,33	0.77	0	48,52,52	0.68	0
14	ATP	F	302	13	32,33,33	0.69	0	48,52,52	0.64	0
14	ATP	K	302	13	32,33,33	0.72	0	48,52,52	0.68	0
14	ATP	L	302	-	32,33,33	0.64	0	48,52,52	0.65	0
14	ATP	A	302	13	32,33,33	0.56	0	48,52,52	0.71	1 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	ATP	J	302	13	-	2/22/38/38	0/3/3/3
14	ATP	B	302	13	-	1/22/38/38	0/3/3/3
14	ATP	E	302	13	-	2/22/38/38	0/3/3/3
14	ATP	C	302	13	-	4/22/38/38	0/3/3/3
14	ATP	D	302	13	-	2/22/38/38	0/3/3/3
14	ATP	G	302	13	-	5/22/38/38	0/3/3/3
14	ATP	H	302	13	-	5/22/38/38	0/3/3/3
14	ATP	I	302	13	-	7/22/38/38	0/3/3/3
14	ATP	F	302	13	-	1/22/38/38	0/3/3/3
14	ATP	K	302	13	-	2/22/38/38	0/3/3/3
14	ATP	L	302	-	-	4/22/38/38	0/3/3/3
14	ATP	A	302	13	-	6/22/38/38	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	302	ATP	C3'-C2'-C1'	2.03	105.30	101.46

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	302	ATP	C5'-O5'-PA-O1A
14	A	302	ATP	C5'-O5'-PA-O2A
14	A	302	ATP	C5'-O5'-PA-O3A
14	A	302	ATP	O4'-C4'-C5'-O5'
14	I	302	ATP	C5'-O5'-PA-O1A
14	I	302	ATP	O4'-C4'-C5'-O5'
14	L	302	ATP	C5'-O5'-PA-O2A
14	L	302	ATP	C5'-O5'-PA-O3A
14	A	302	ATP	C3'-C4'-C5'-O5'
14	C	302	ATP	C3'-C4'-C5'-O5'
14	H	302	ATP	C3'-C4'-C5'-O5'
14	C	302	ATP	O4'-C4'-C5'-O5'
14	H	302	ATP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
14	I	302	ATP	C3'-C4'-C5'-O5'
14	G	302	ATP	O4'-C4'-C5'-O5'
14	G	302	ATP	C3'-C4'-C5'-O5'
14	H	302	ATP	C4'-C5'-O5'-PA
14	D	302	ATP	PA-O3A-PB-O1B
14	G	302	ATP	PA-O3A-PB-O2B
14	H	302	ATP	PA-O3A-PB-O2B
14	I	302	ATP	PA-O3A-PB-O1B
14	I	302	ATP	PA-O3A-PB-O2B
14	J	302	ATP	O4'-C4'-C5'-O5'
14	I	302	ATP	C5'-O5'-PA-O2A
14	I	302	ATP	C5'-O5'-PA-O3A
14	L	302	ATP	C5'-O5'-PA-O1A
14	D	302	ATP	PA-O3A-PB-O2B
14	E	302	ATP	PA-O3A-PB-O2B
14	H	302	ATP	PA-O3A-PB-O1B
14	J	302	ATP	PA-O3A-PB-O2B
14	G	302	ATP	C4'-C5'-O5'-PA
14	B	302	ATP	O4'-C4'-C5'-O5'
14	C	302	ATP	PA-O3A-PB-O1B
14	C	302	ATP	PA-O3A-PB-O2B
14	K	302	ATP	C3'-C4'-C5'-O5'
14	F	302	ATP	O4'-C4'-C5'-O5'
14	A	302	ATP	C2'-C1'-N9-C8
14	E	302	ATP	O4'-C4'-C5'-O5'
14	G	302	ATP	PA-O3A-PB-O1B
14	L	302	ATP	PA-O3A-PB-O2B
14	K	302	ATP	O4'-C4'-C5'-O5'

There are no ring outliers.

12 monomers are involved in 43 short contacts:

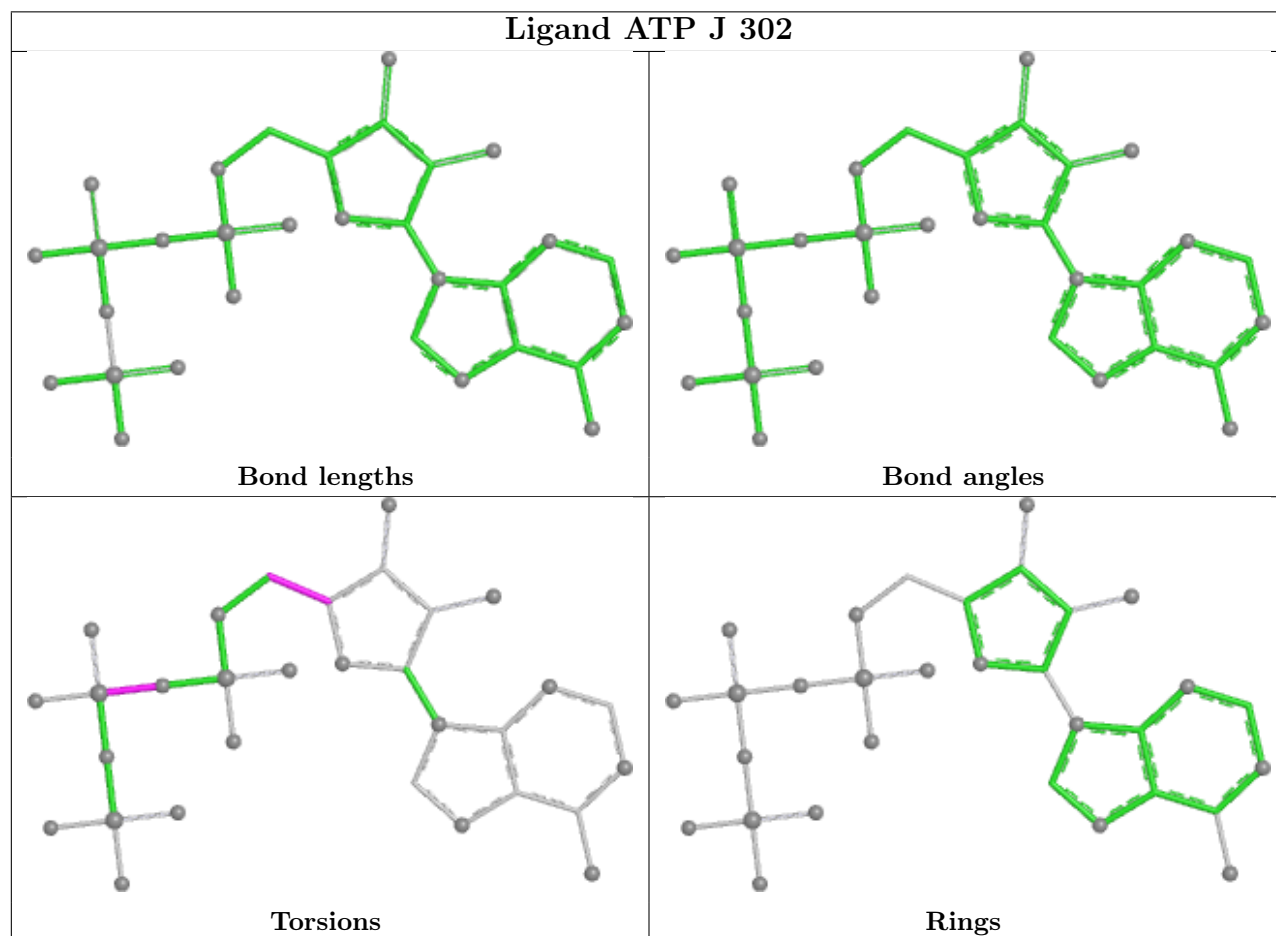
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	J	302	ATP	2	0
14	B	302	ATP	8	0
14	E	302	ATP	2	0
14	C	302	ATP	4	0
14	D	302	ATP	5	0
14	G	302	ATP	2	0
14	H	302	ATP	3	0
14	I	302	ATP	3	0
14	F	302	ATP	3	0

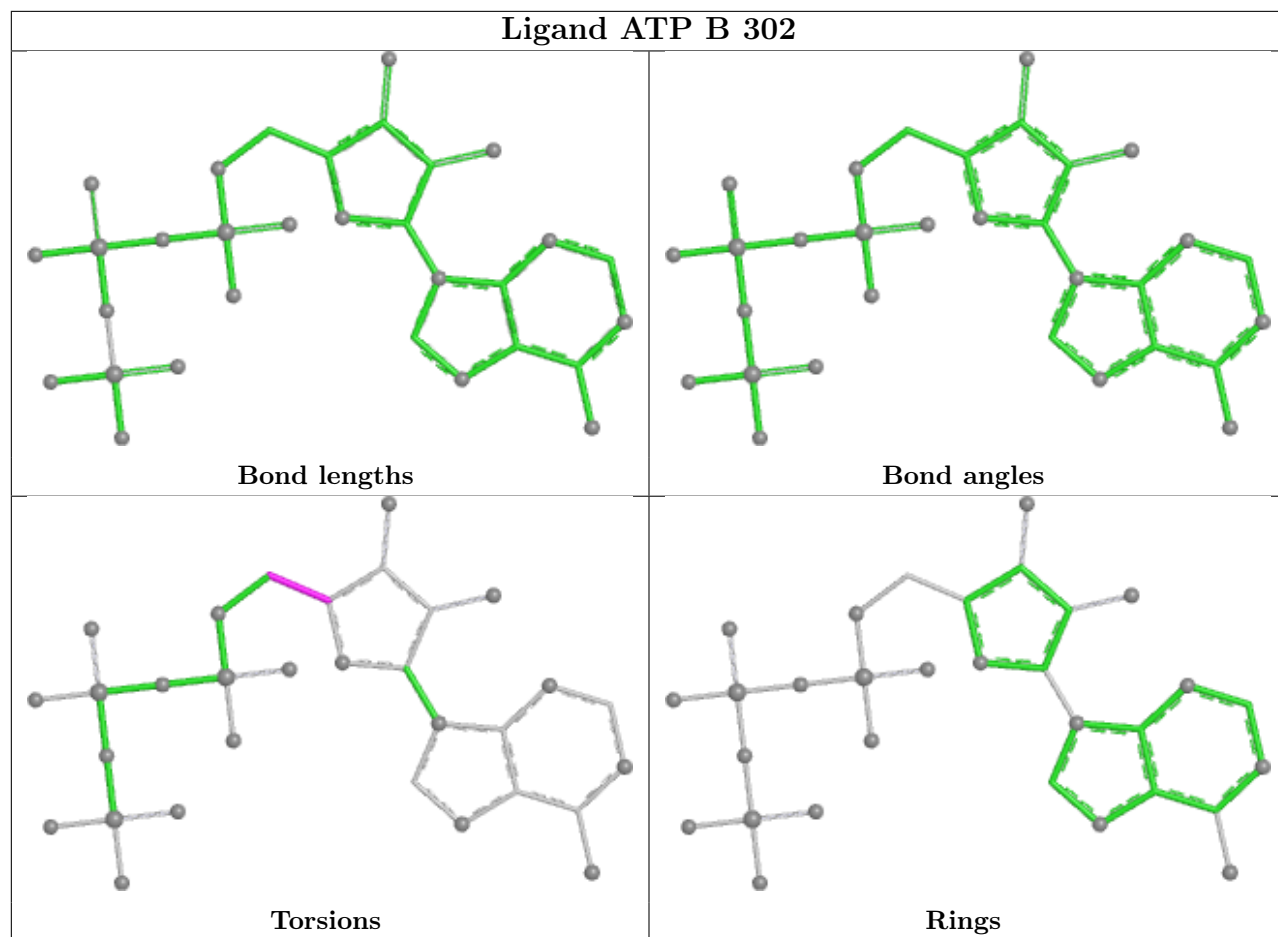
Continued on next page...

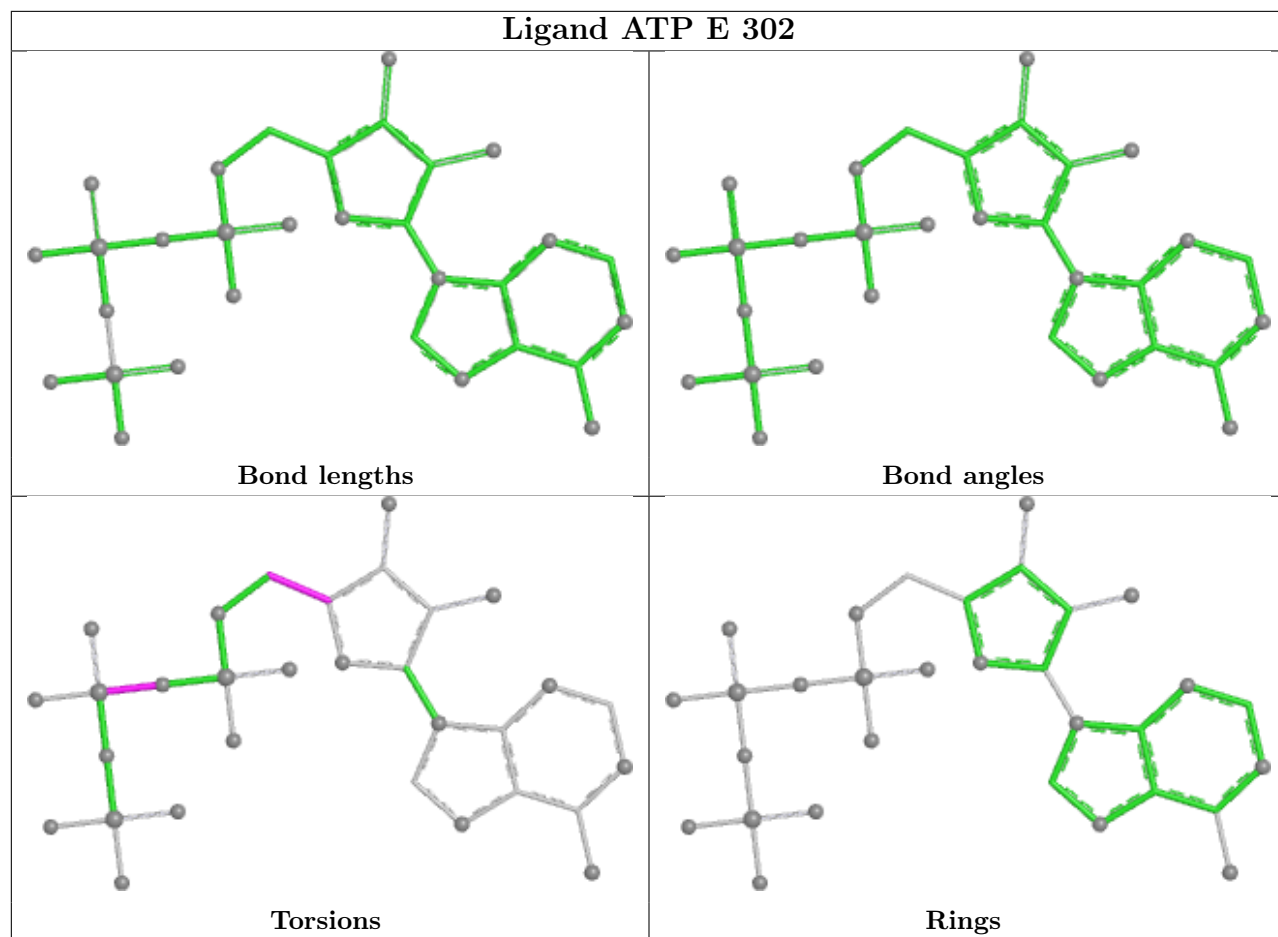
Continued from previous page...

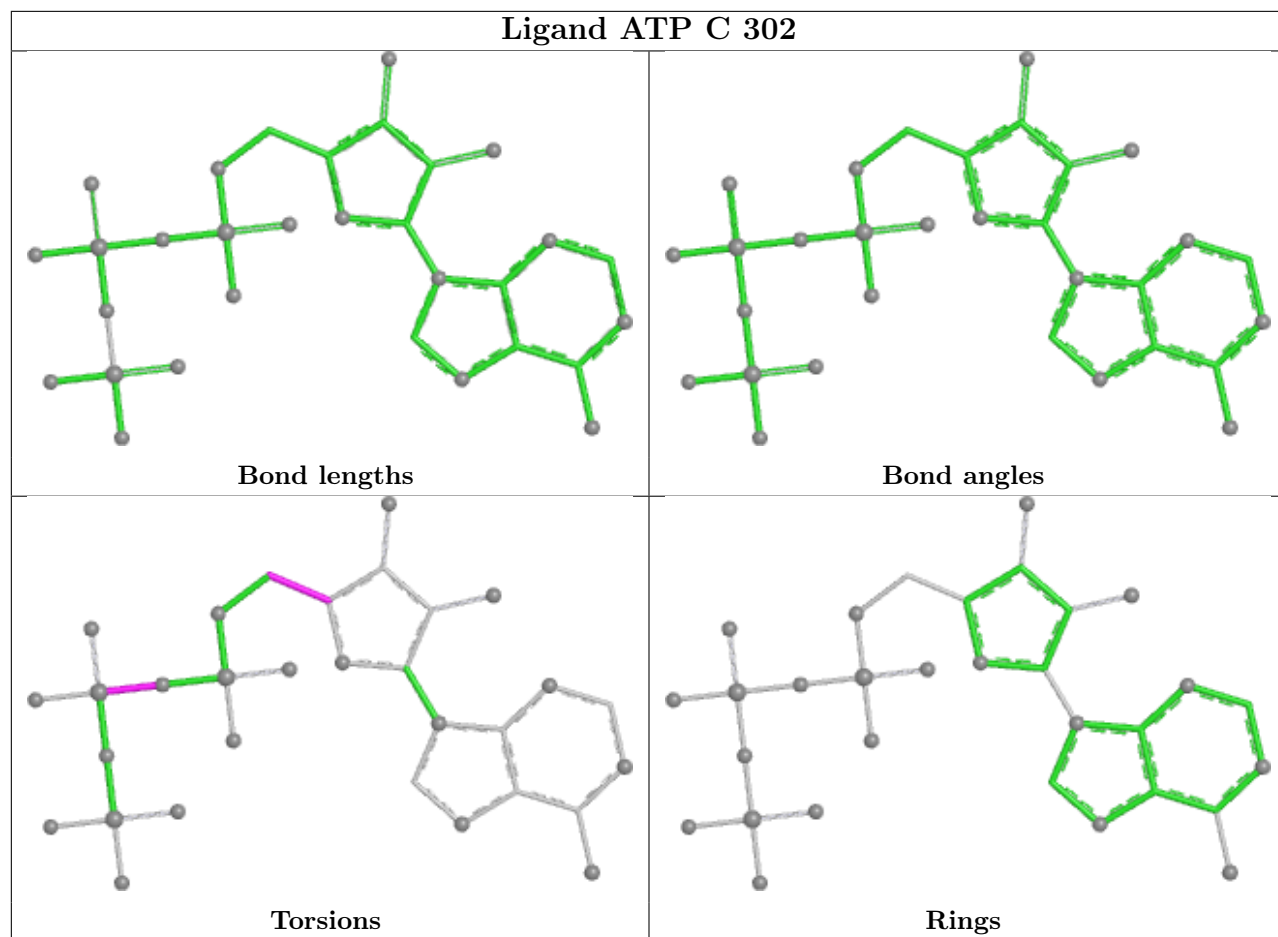
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	K	302	ATP	1	0
14	L	302	ATP	7	0
14	A	302	ATP	3	0

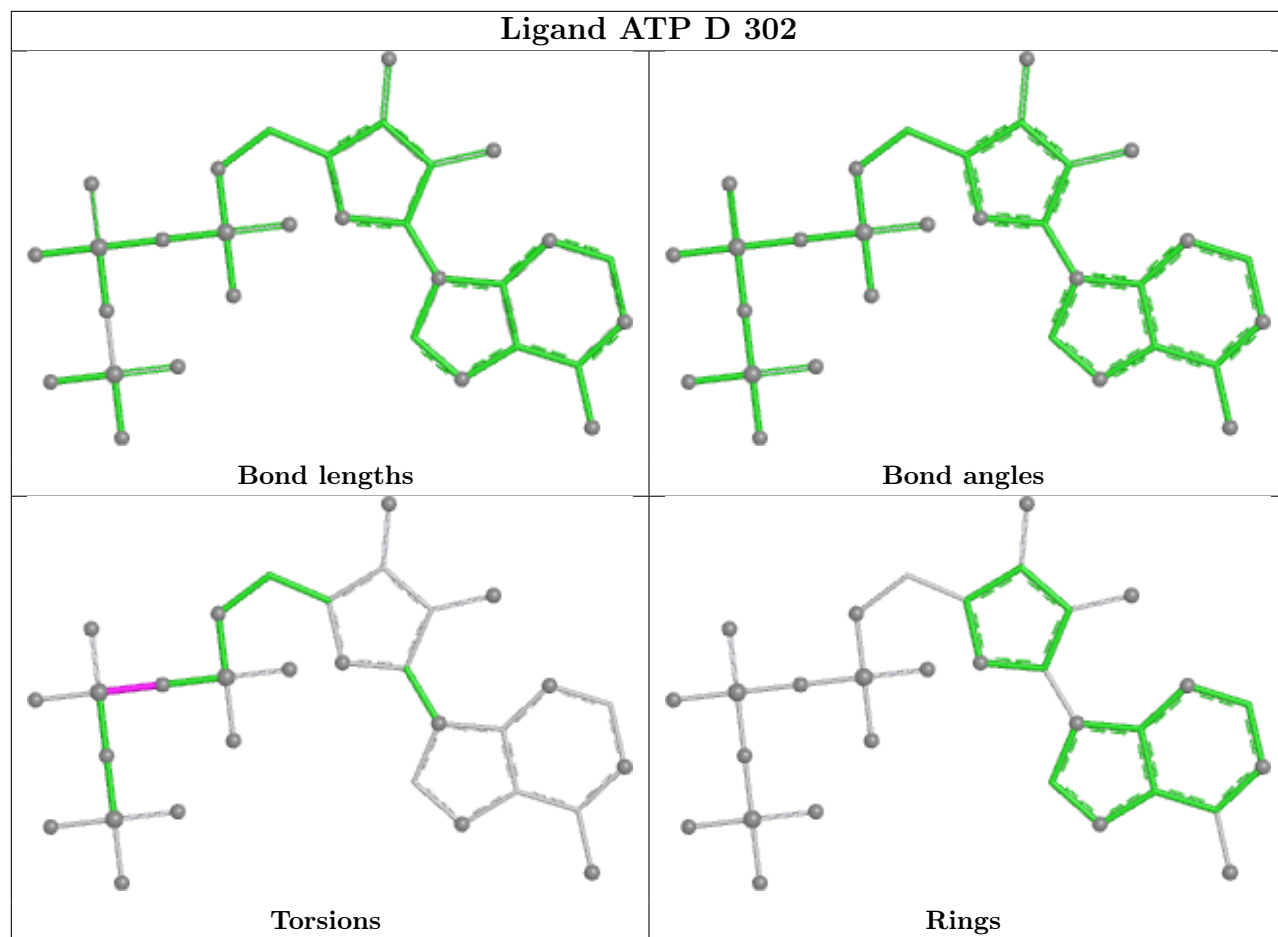
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

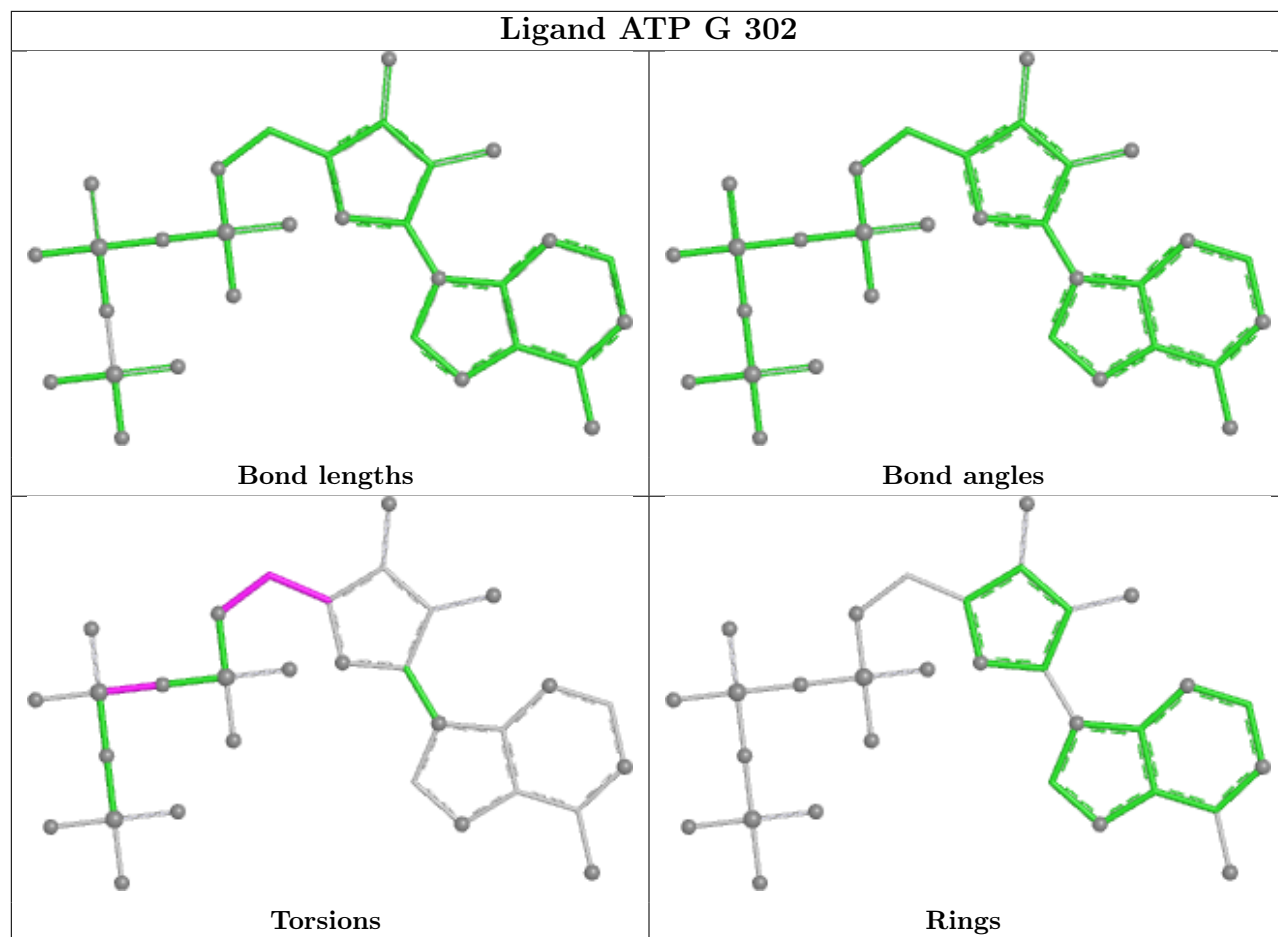


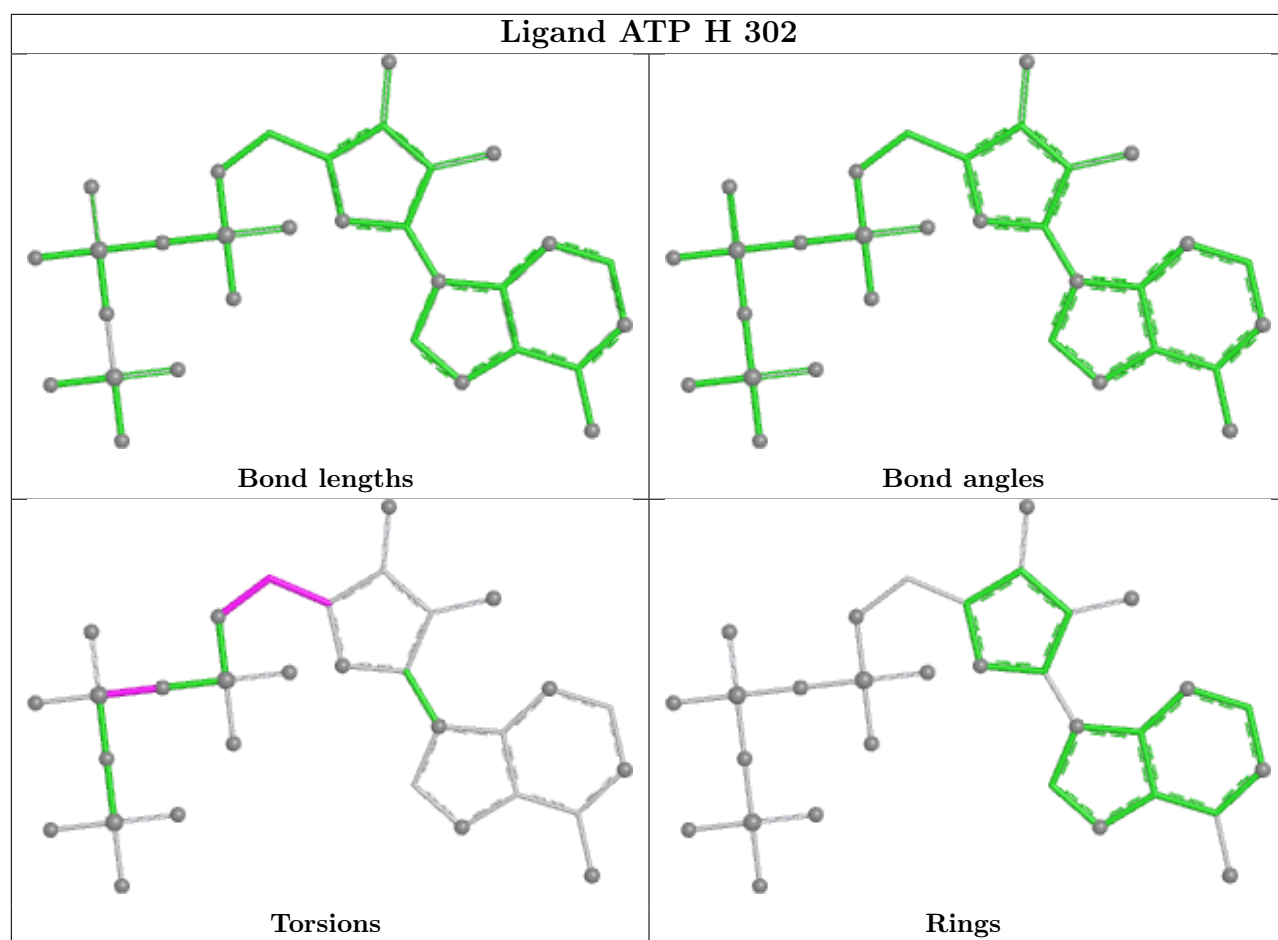


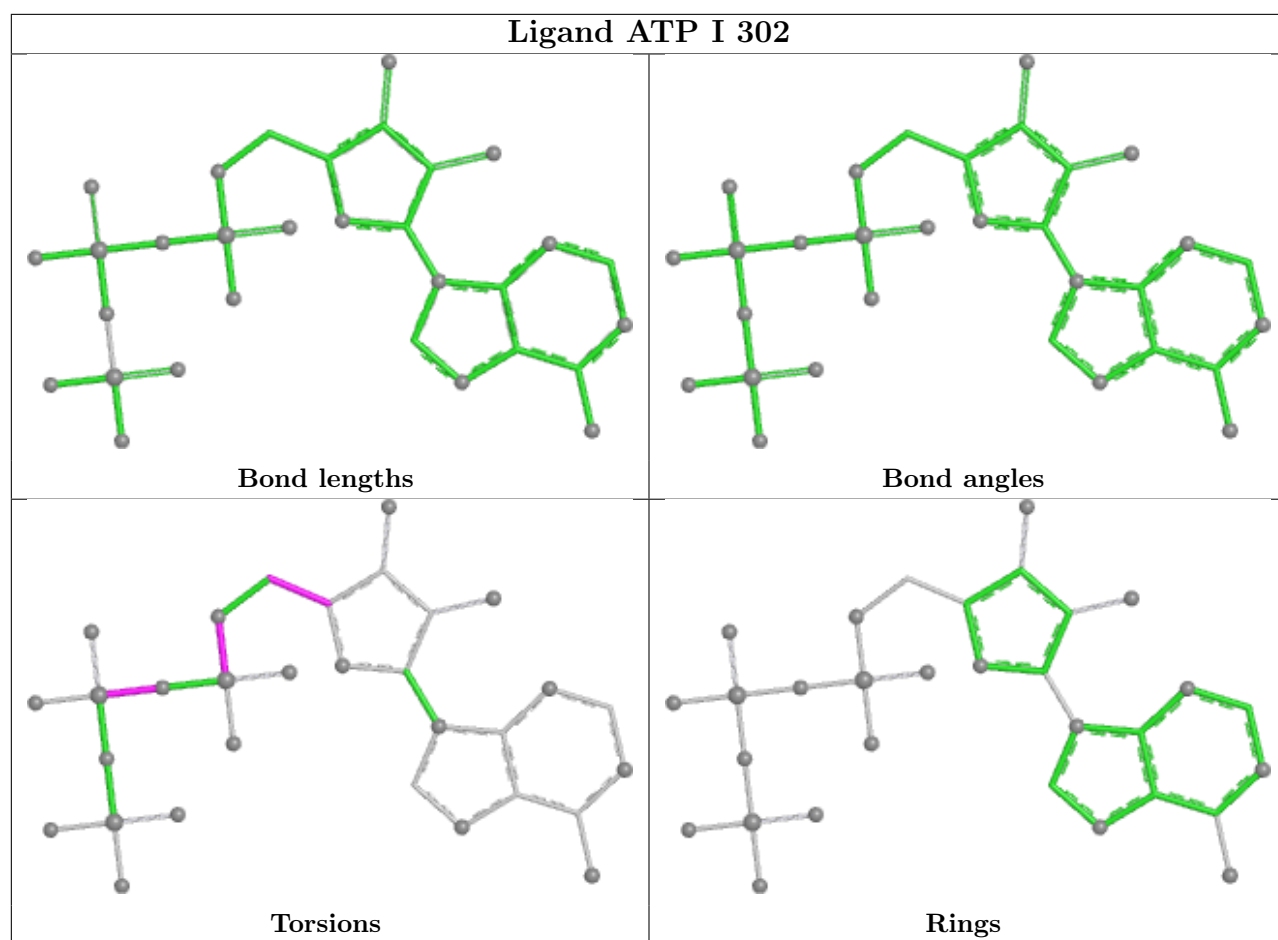


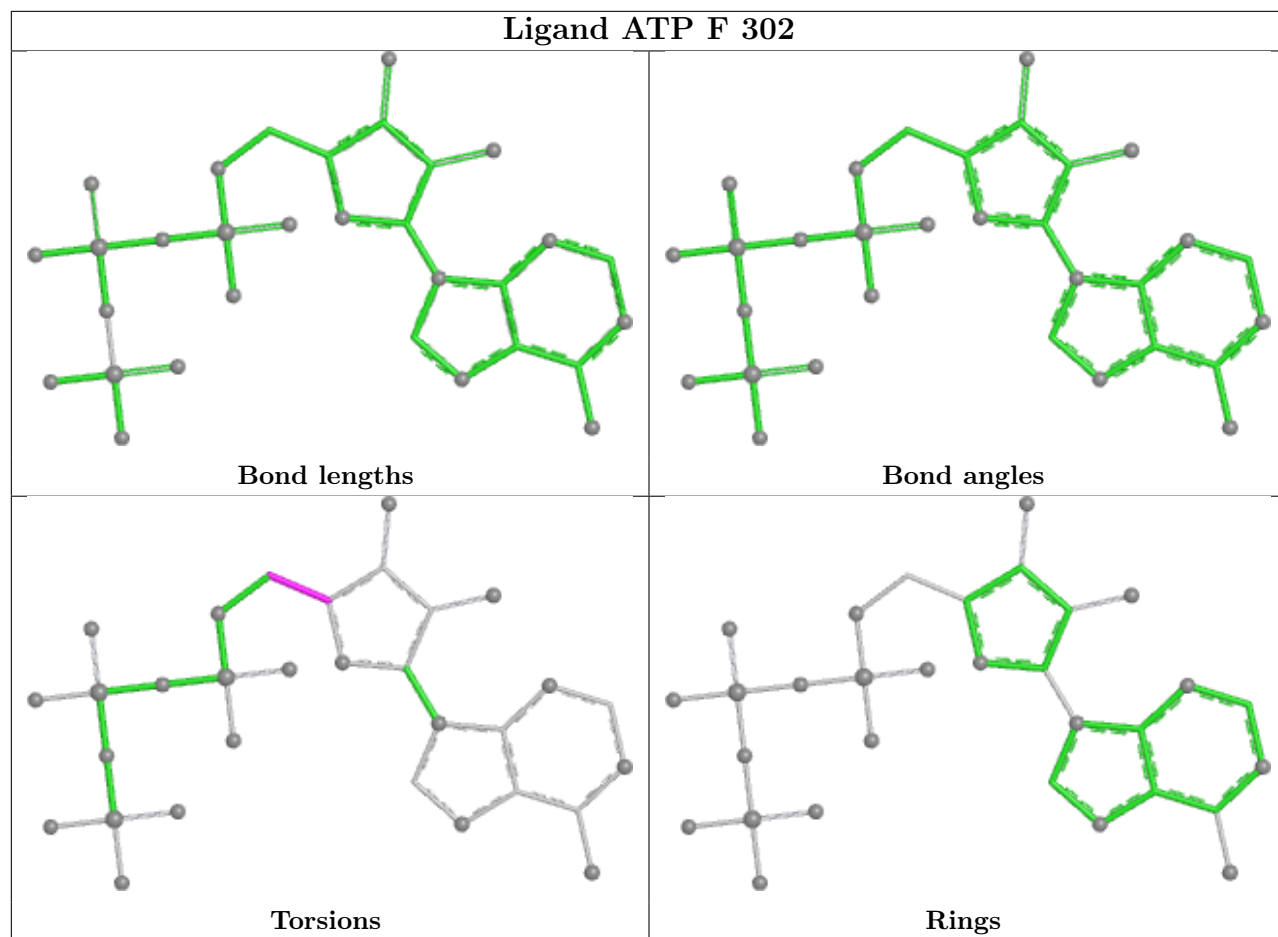


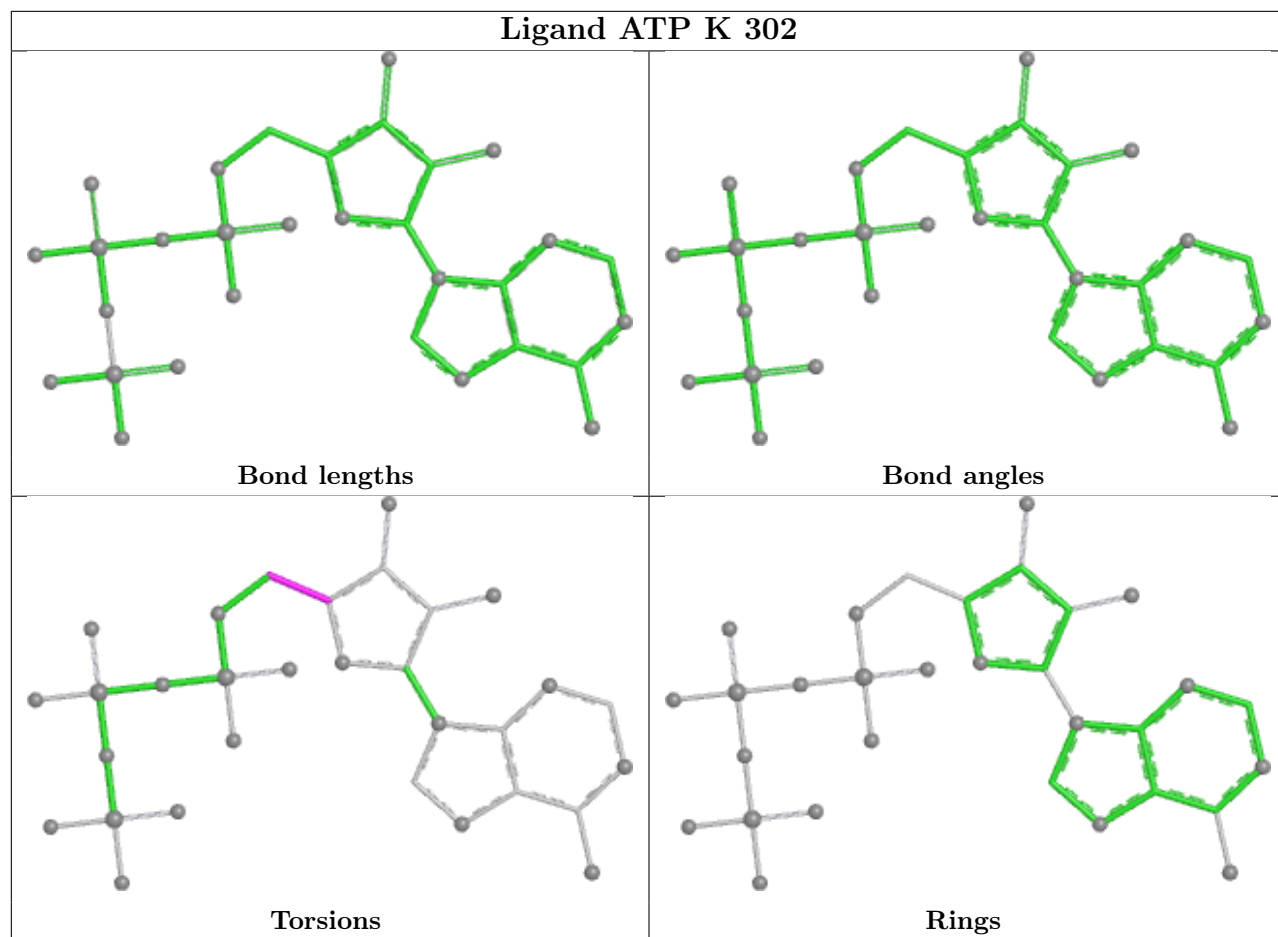


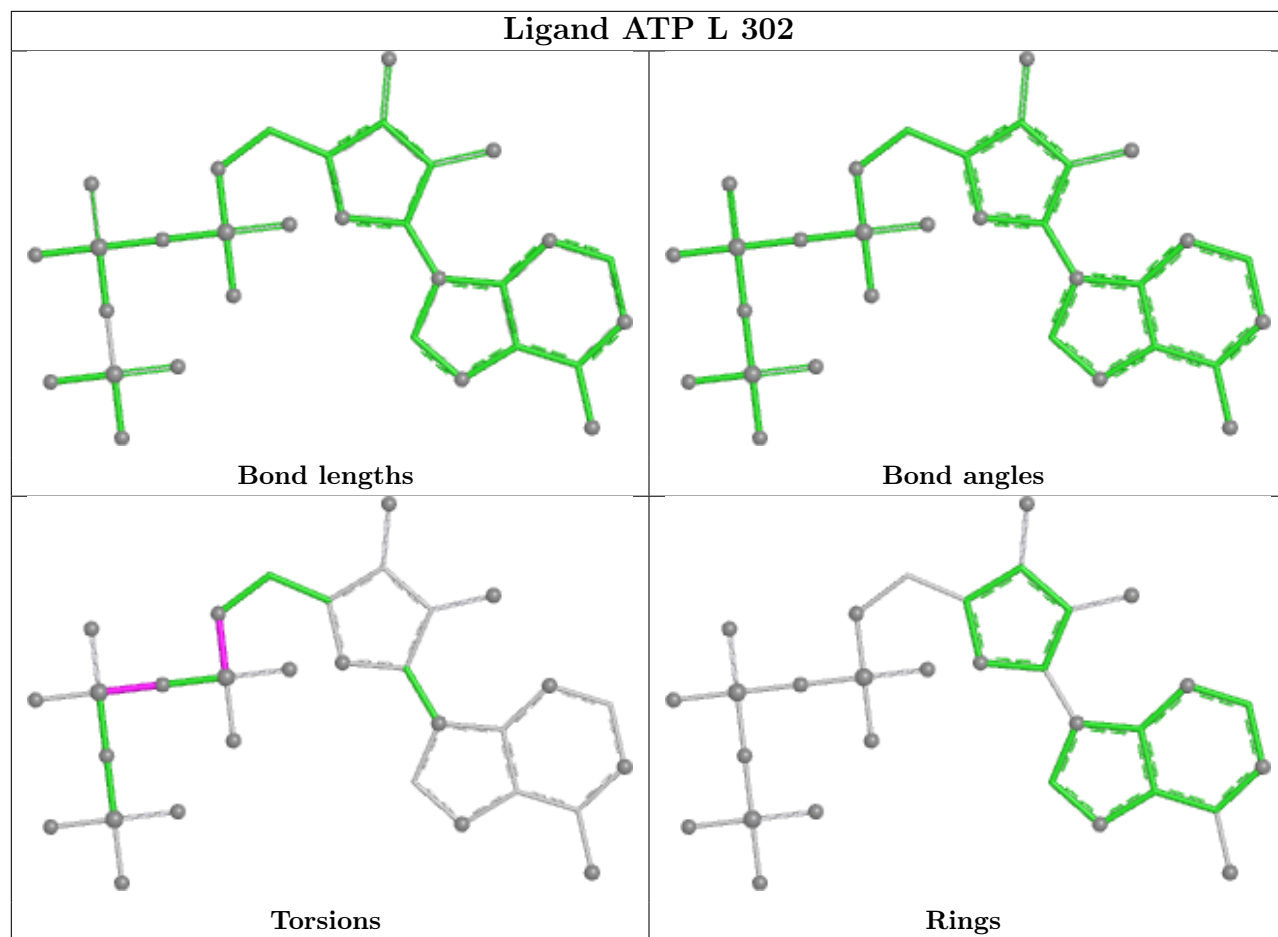


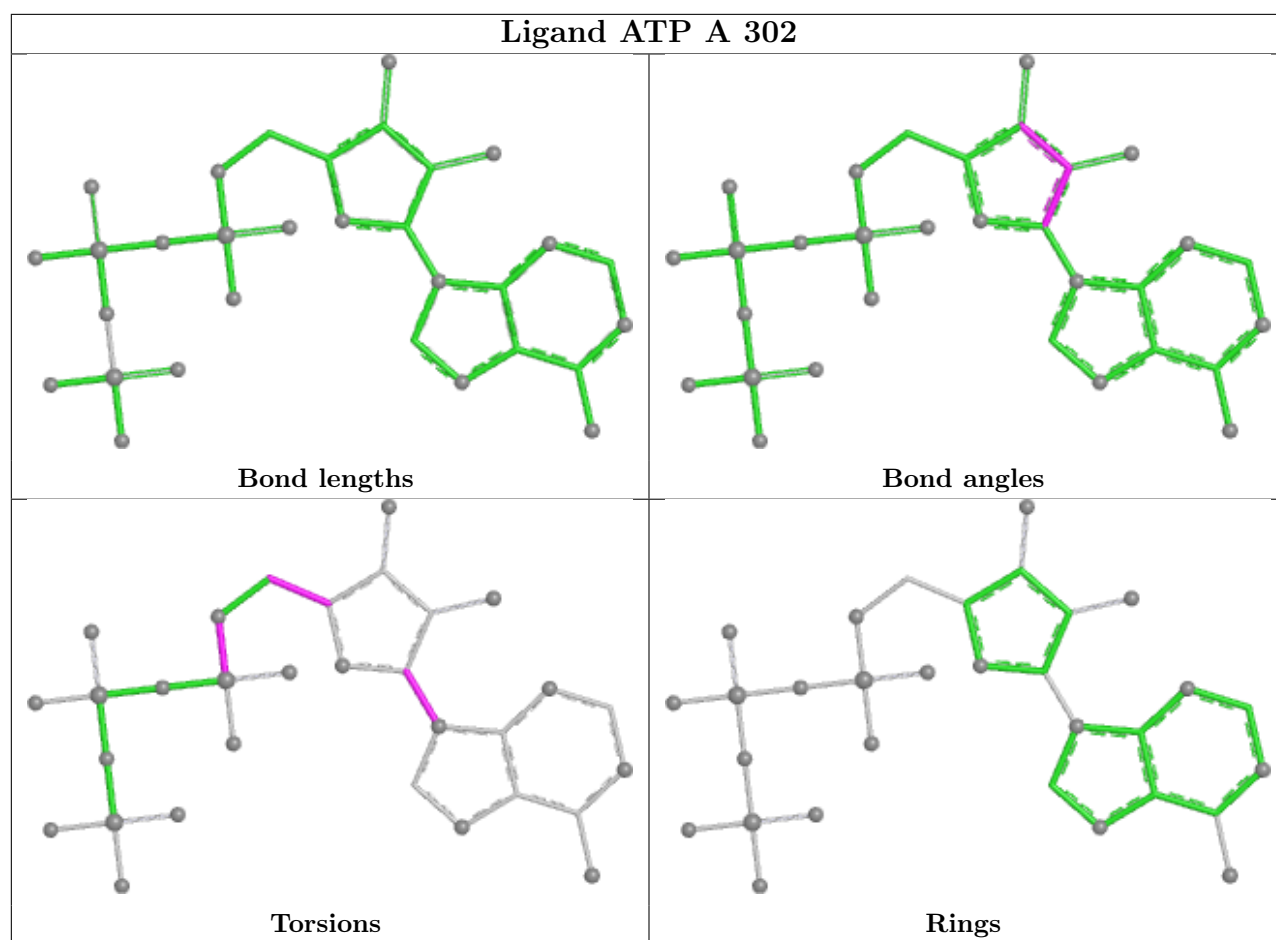












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

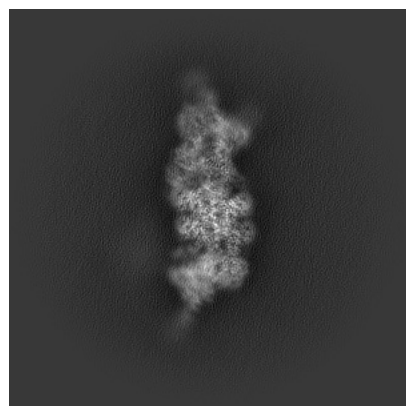
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27971. These allow visual inspection of the internal detail of the map and identification of artifacts.

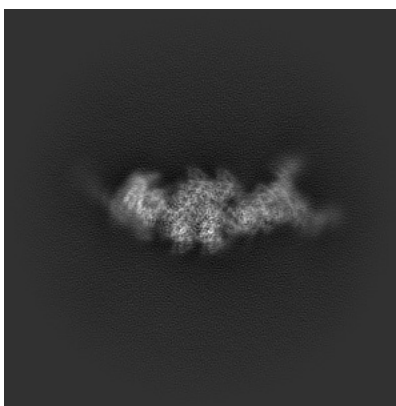
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

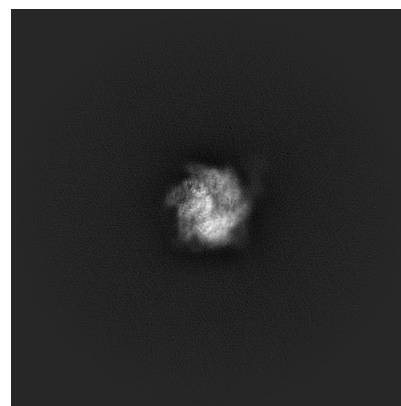
6.1.1 Primary map



X

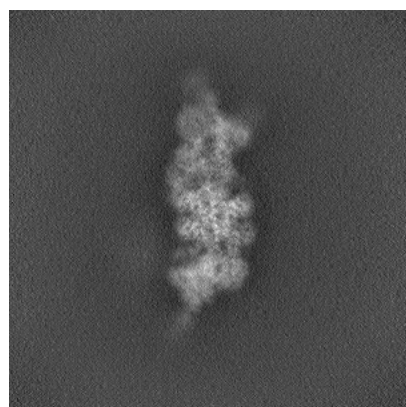


Y

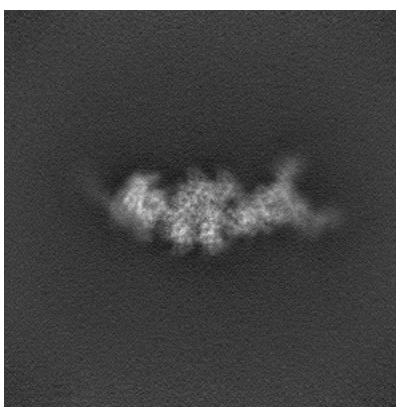


Z

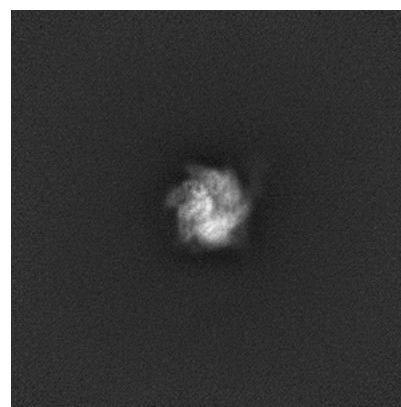
6.1.2 Raw map



X



Y

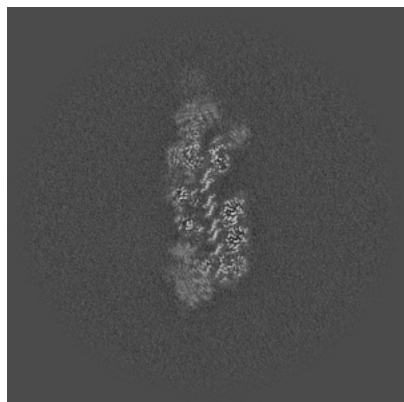


Z

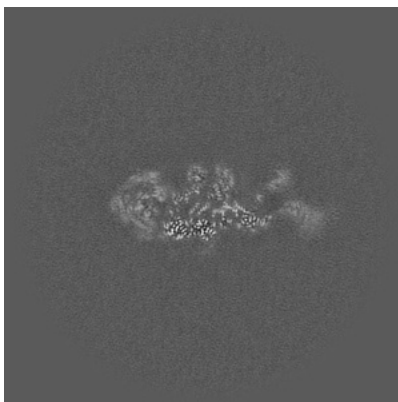
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

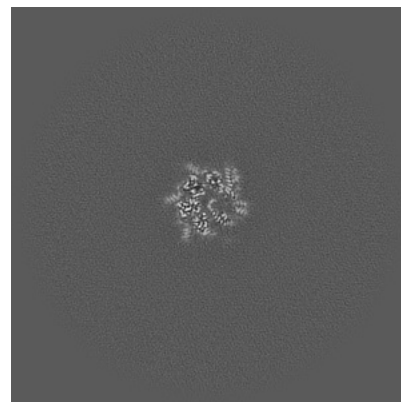
6.2.1 Primary map



X Index: 270

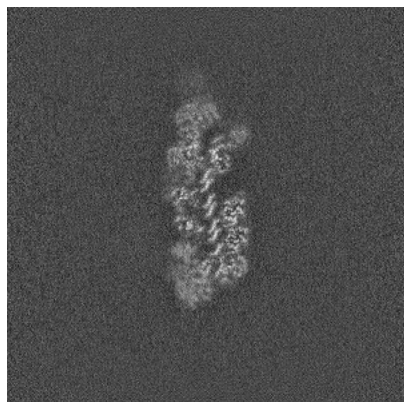


Y Index: 270

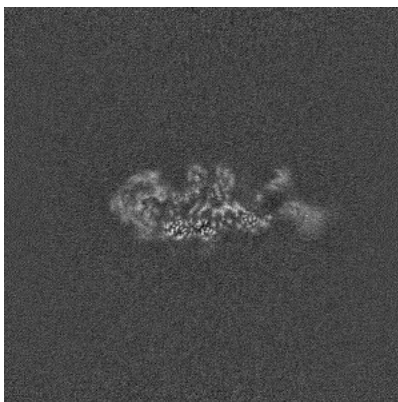


Z Index: 270

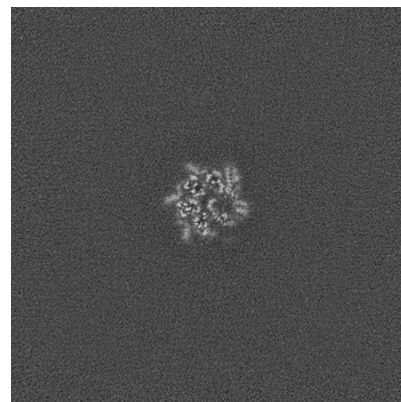
6.2.2 Raw map



X Index: 270



Y Index: 270

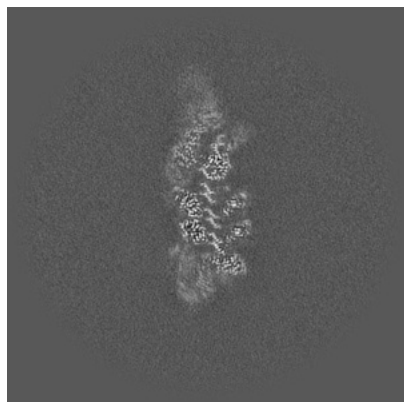


Z Index: 270

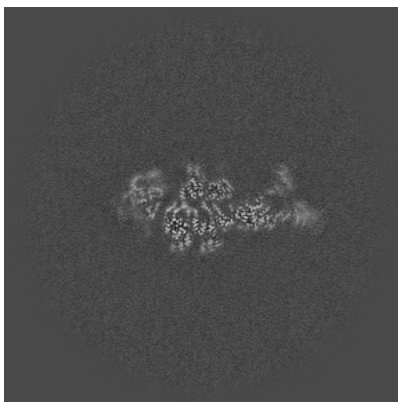
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

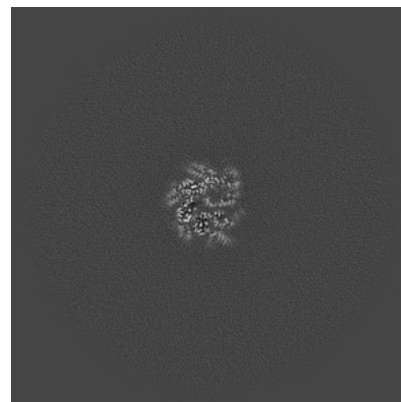
6.3.1 Primary map



X Index: 264

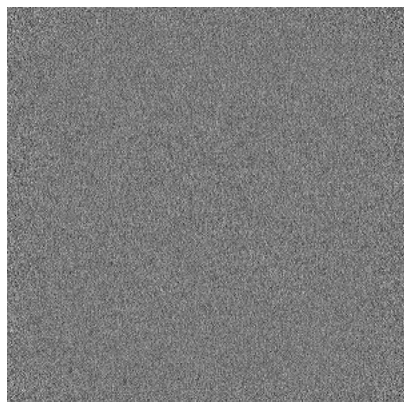


Y Index: 278

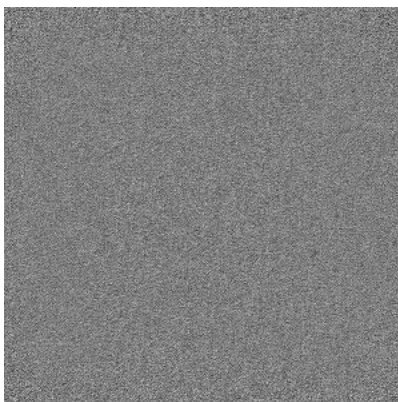


Z Index: 277

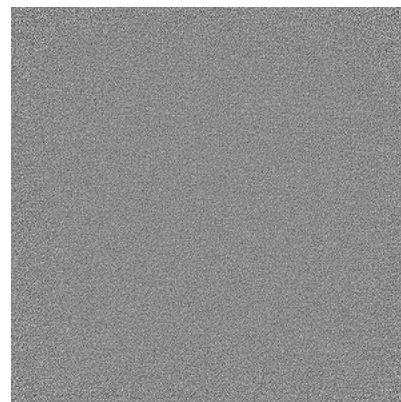
6.3.2 Raw map



X Index: 0



Y Index: 0

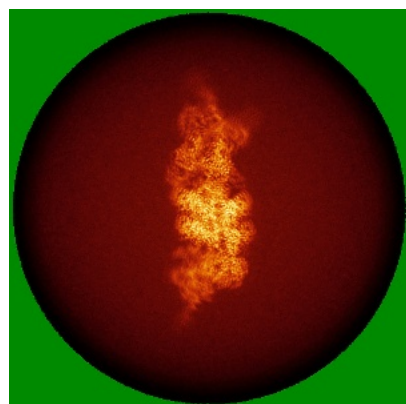


Z Index: 0

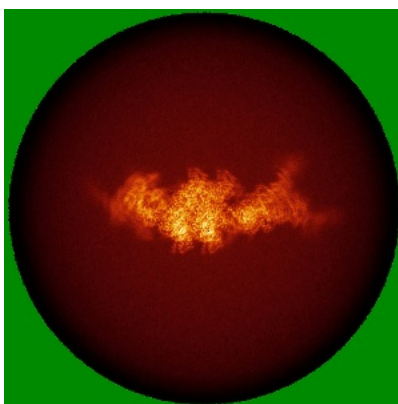
The images above show the largest variance slices of the map in three orthogonal directions.

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

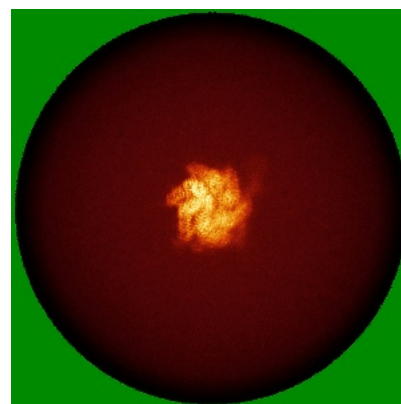
6.4.1 Primary map



X

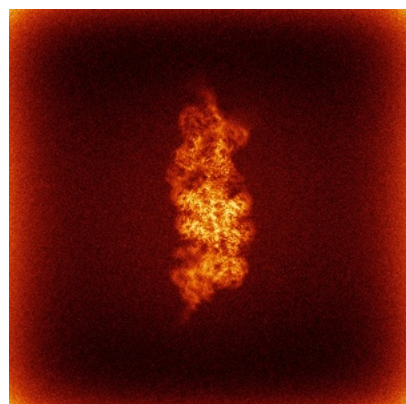


Y

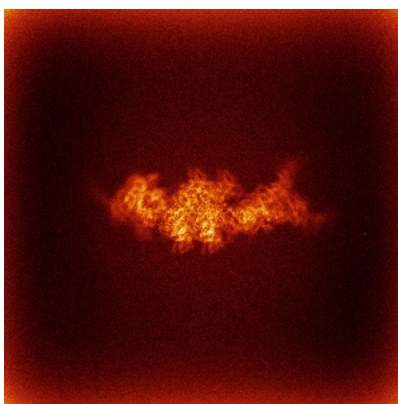


Z

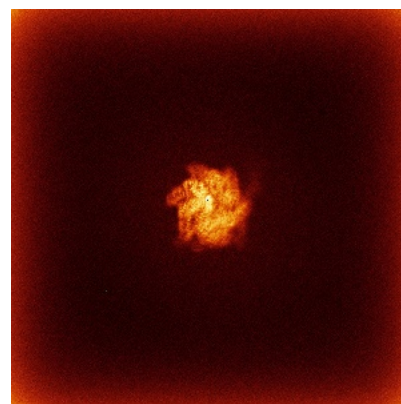
6.4.2 Raw map



X



Y

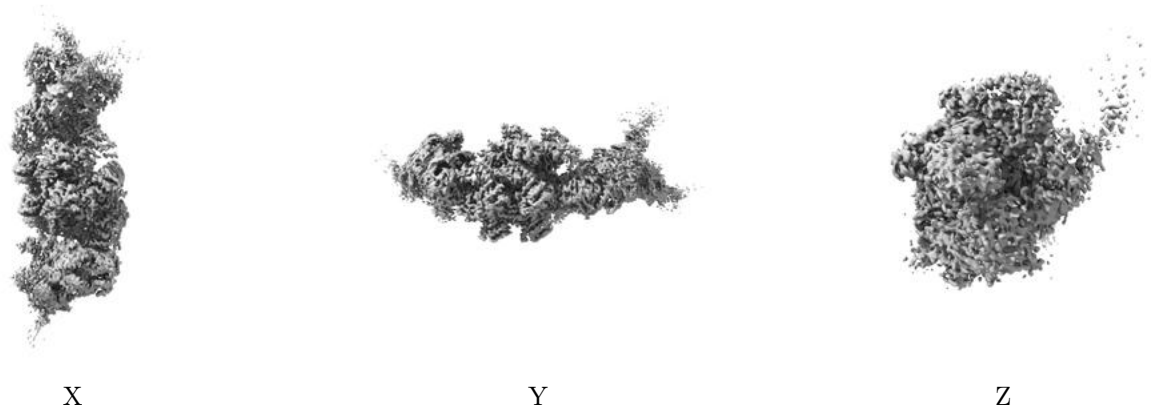


Z

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

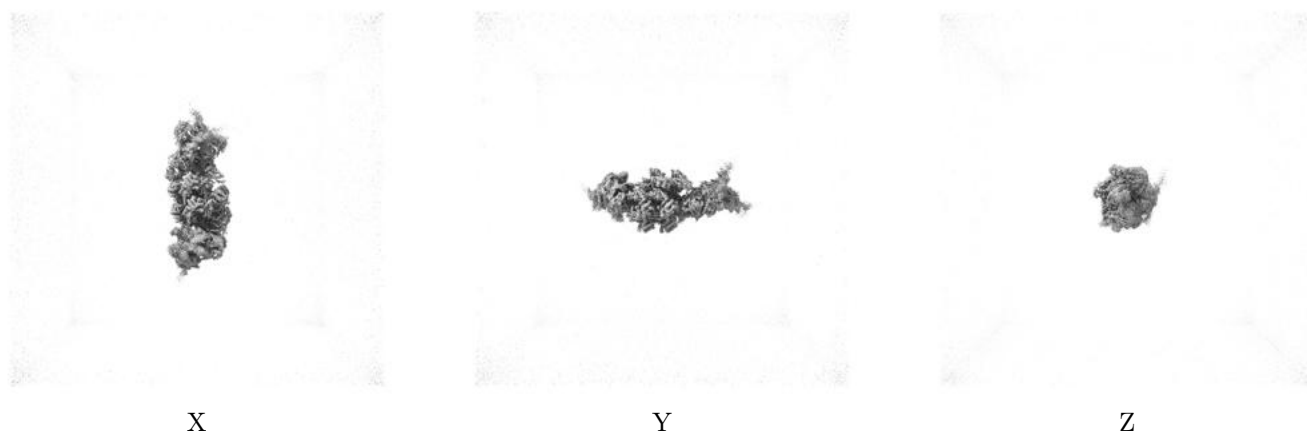
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

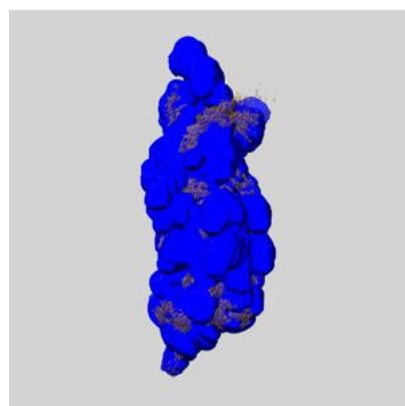
6.6 Mask visualisation [i](#)

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

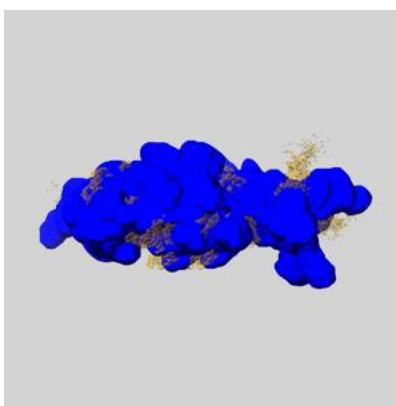
A mask typically either:

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

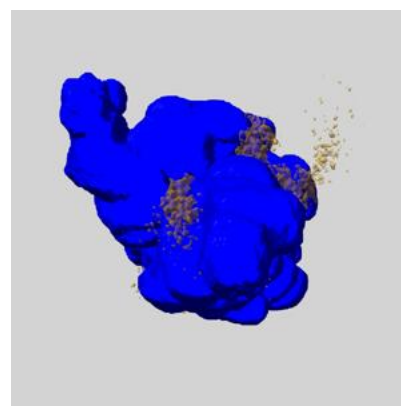
6.6.1 emd_27971_msk_1.map [i](#)



X



Y

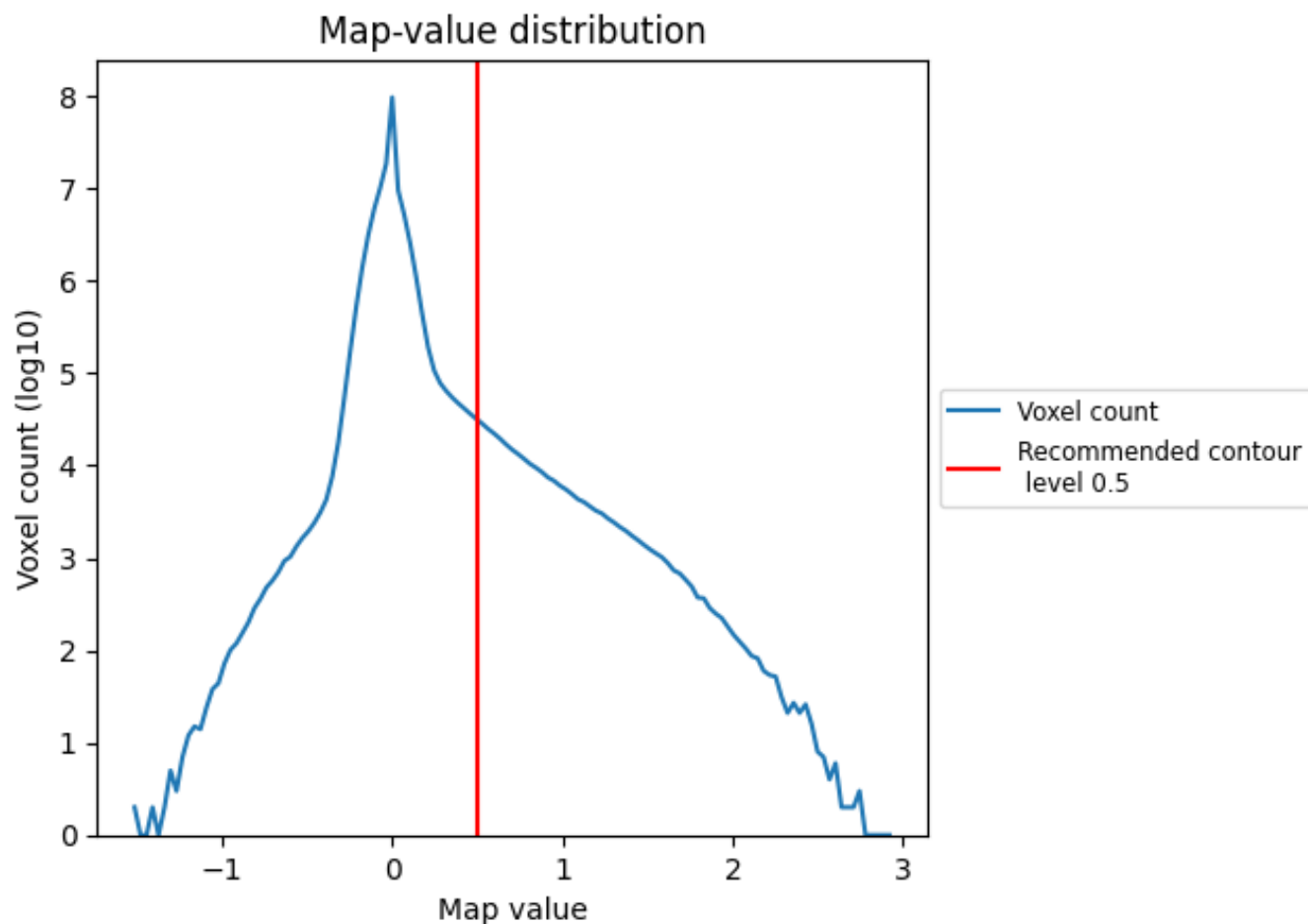


Z

7 Map analysis [i](#)

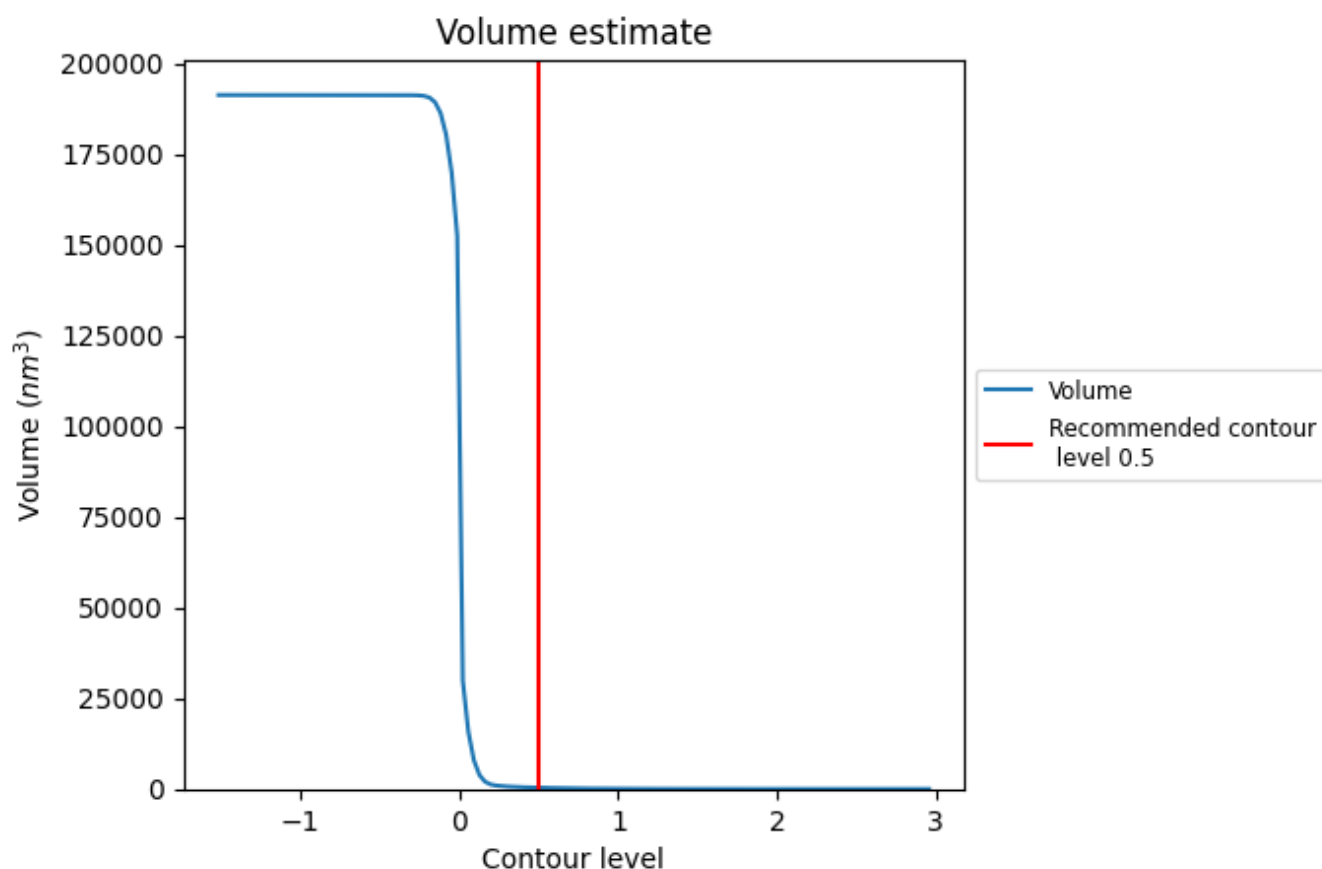
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

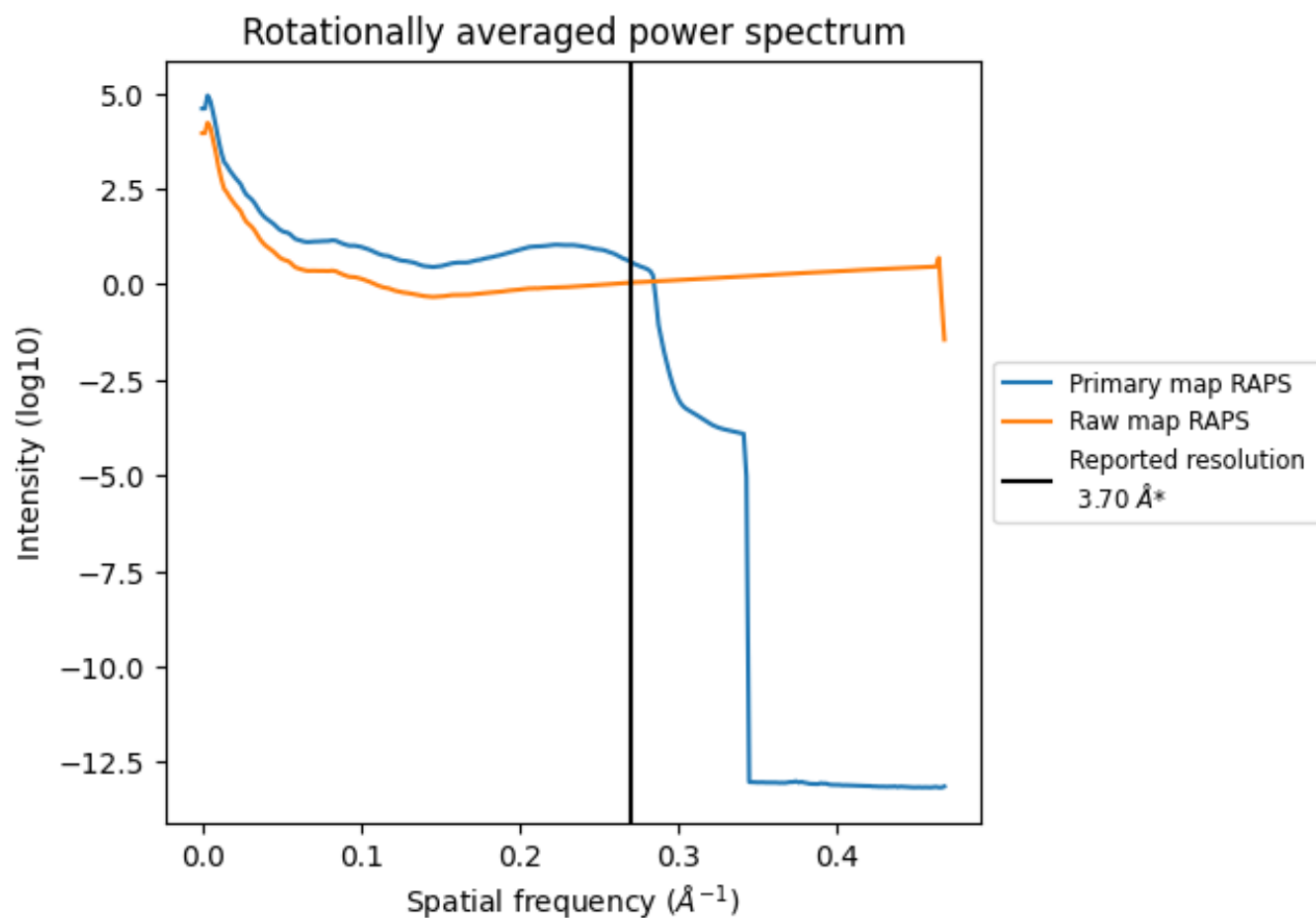
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 338 nm³; this corresponds to an approximate mass of 305 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 ⓘ

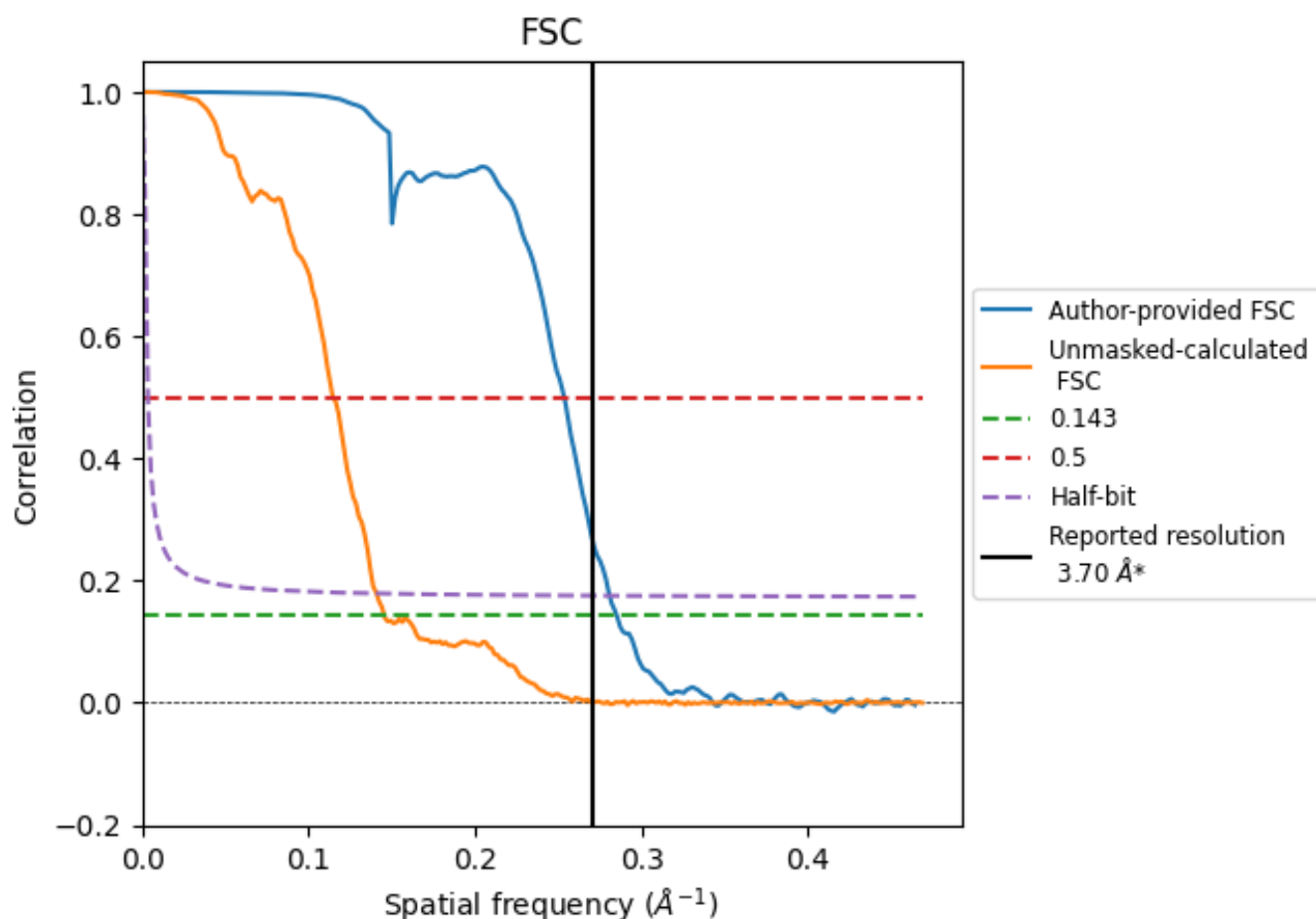


*Reported resolution corresponds to spatial frequency of 0.270 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.270 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

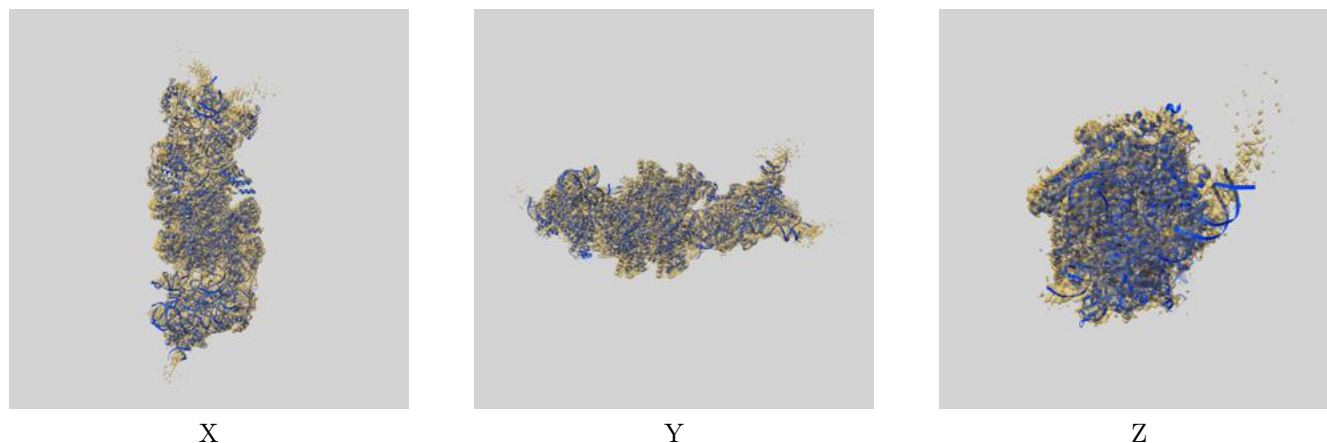
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.51	3.94	3.56
Unmasked-calculated*	6.88	8.73	7.10

*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 6.88 differs from the reported value 3.7 by more than 10 %

9 Map-model fit [i](#)

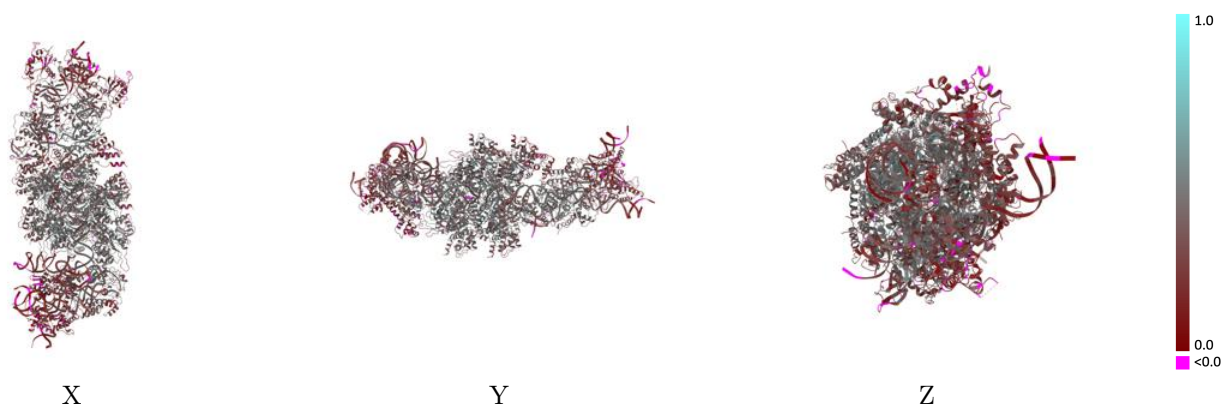
This section contains information regarding the fit between EMDB map EMD-27971 and PDB model 8EA3. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



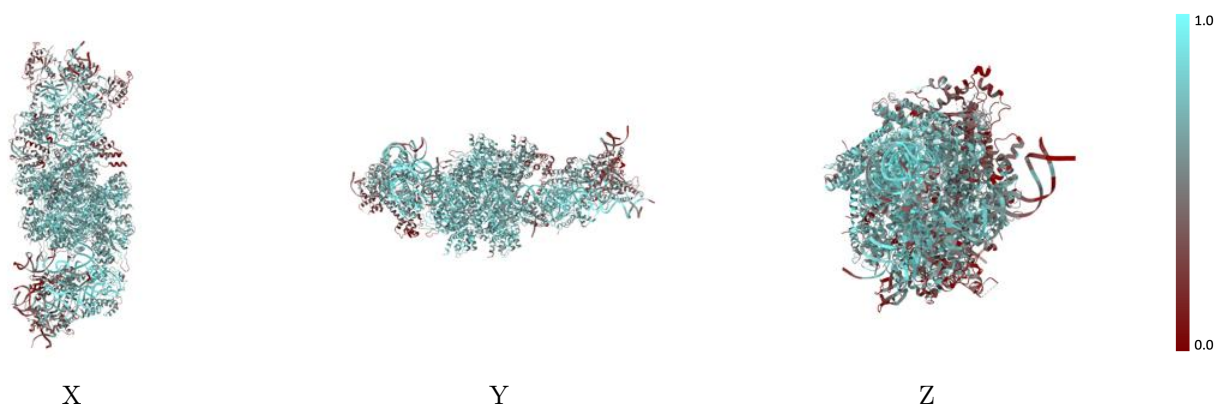
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



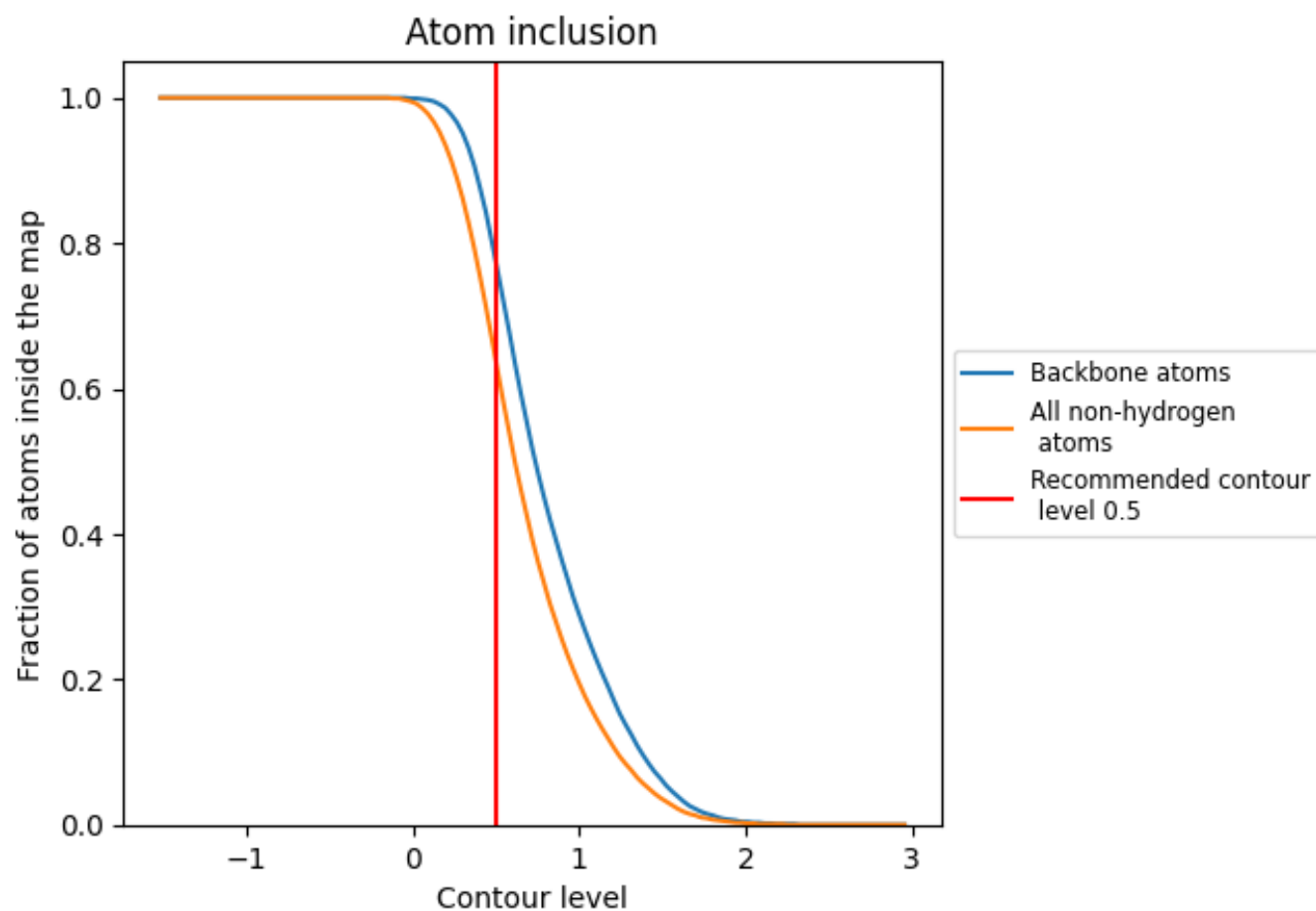
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 64% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6380	 0.3560
1	 0.7490	 0.3400
2	 0.6240	 0.2730
3	 0.7850	 0.3670
4	 0.7660	 0.3160
5	 0.7770	 0.3190
6	 0.6580	 0.2370
7	 0.6460	 0.2510
A	 0.5040	 0.3410
B	 0.6610	 0.3940
C	 0.7520	 0.4260
D	 0.7680	 0.4460
E	 0.7640	 0.4410
F	 0.7120	 0.4120
G	 0.7100	 0.4080
H	 0.7070	 0.4230
I	 0.7160	 0.4220
J	 0.7280	 0.4350
K	 0.7780	 0.4540
L	 0.6670	 0.4160
O	 0.3840	 0.2080
Q	 0.7800	 0.4330
S	 0.6090	 0.3230
W	 0.6700	 0.4100
X	 0.5680	 0.3530
Y	 0.4410	 0.2620
Z	 0.4410	 0.2690
w	 0.4840	 0.3620
x	 0.3060	 0.2780
y	 0.3950	 0.3500
z	 0.3060	 0.2850

