



Full wwPDB EM Validation Report ⓘ

Nov 29, 2022 – 01:39 AM EST

PDB ID : 7UFM
EMDB ID : EMD-26477
Title : VchTnsC AAA+ with DNA (double heptamer)
Authors : Fernandez, I.S.; Sternberg, S.H.
Deposited on : 2022-03-22
Resolution : 3.90 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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

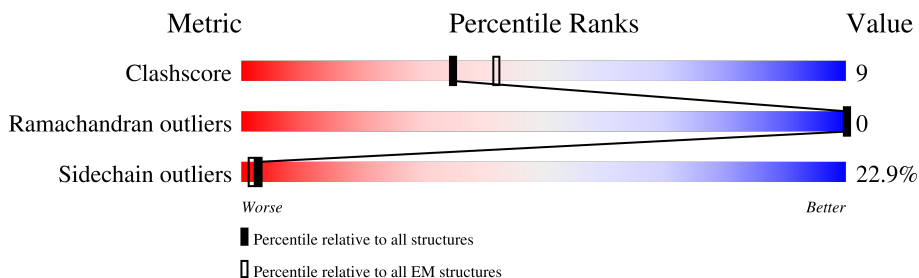
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 Å.

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






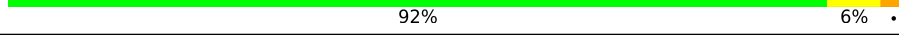

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	311	65% 29% 5% •
1	B	311	64% 29% 5% •
1	C	311	64% 30% • •
1	D	311	64% 30% 5% •
1	E	311	65% 29% 5% •
1	F	311	65% 28% 5% •
1	G	311	63% 30% 6% •
1	H	311	64% 30% 5% •
1	I	311	63% 30% 5% •

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Mol	Chain	Length	Quality of chain
1	J	311	 64% 29% 5% .
1	K	311	 64% 30% 5% .
1	L	311	 64% 29% 5% .
1	M	311	 63% 31% 5% .
1	N	311	 65% 28% 5% .
2	O	36	 92% 6% .
3	P	36	 89% 11%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 36392 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called VchTnsC.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	311	2463	1567	426	459	11	0	0
1	B	311	2463	1567	426	459	11	0	0
1	C	311	2463	1567	426	459	11	0	0
1	D	311	2463	1567	426	459	11	0	0
1	E	311	2463	1567	426	459	11	0	0
1	F	311	2463	1567	426	459	11	0	0
1	G	311	2463	1567	426	459	11	0	0
1	H	311	2463	1567	426	459	11	0	0
1	I	311	2463	1567	426	459	11	0	0
1	J	311	2463	1567	426	459	11	0	0
1	K	311	2463	1567	426	459	11	0	0
1	L	311	2463	1567	426	459	11	0	0
1	M	311	2463	1567	426	459	11	0	0
1	N	311	2463	1567	426	459	11	0	0

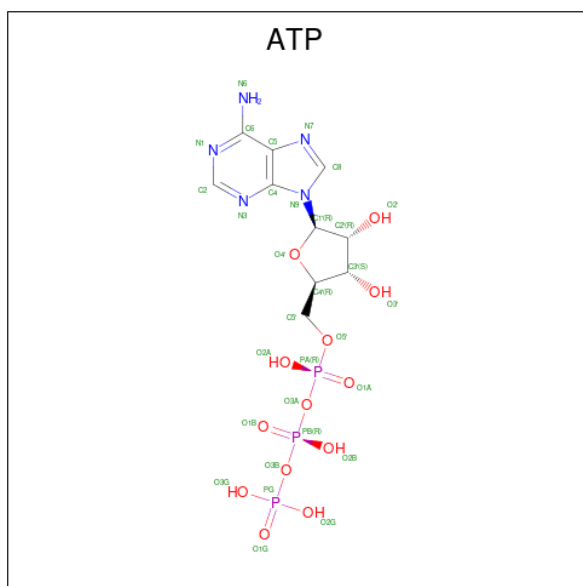
- Molecule 2 is a DNA chain called DNA (36-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	O	36	737	350	139	212	36	0	0

- Molecule 3 is a DNA chain called DNA (36-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	P	36	739	352	131	220	36	0	0

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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

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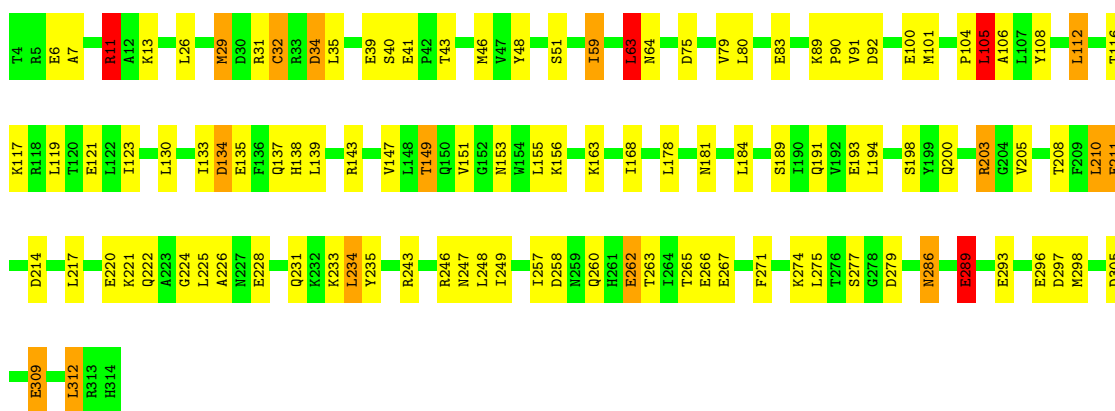
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
4	J	1	Total 31	10	5	13	3	0
4	K	1	Total 31	10	5	13	3	0
4	L	1	Total 31	10	5	13	3	0
4	M	1	Total 31	10	5	13	3	0
4	N	1	Total 31	10	5	13	3	0

3 Residue-property plots

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

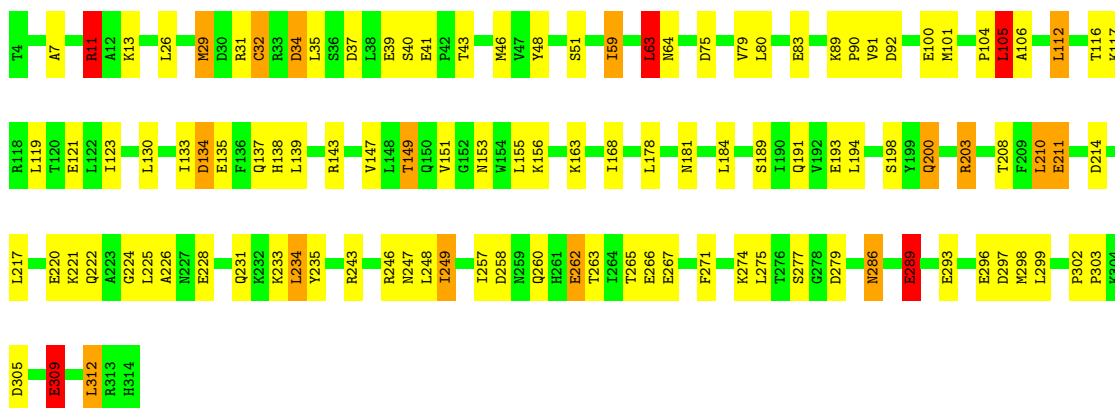
- Molecule 1: VchTnsC

Chain A: 



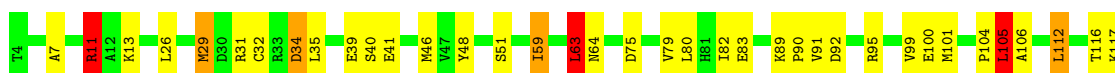
- Molecule 1: VchTnsC

Chain B: 



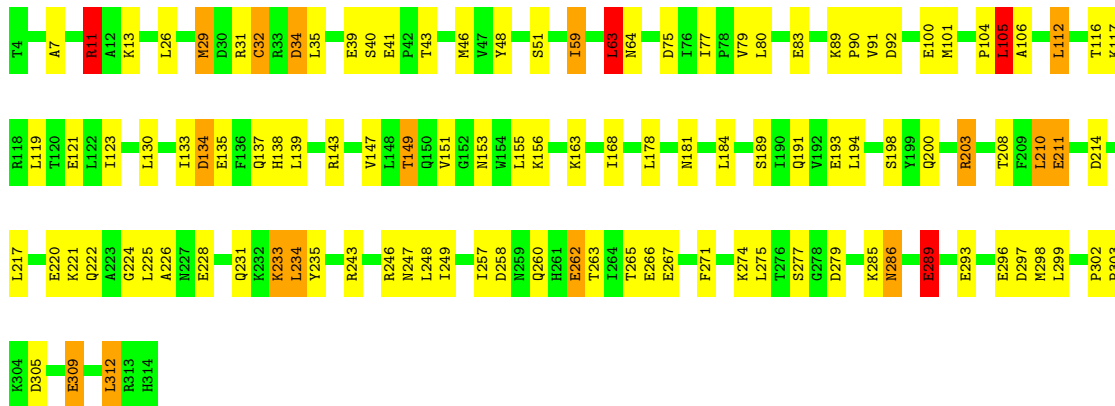
- Molecule 1: VchTnsC

Chain C: 

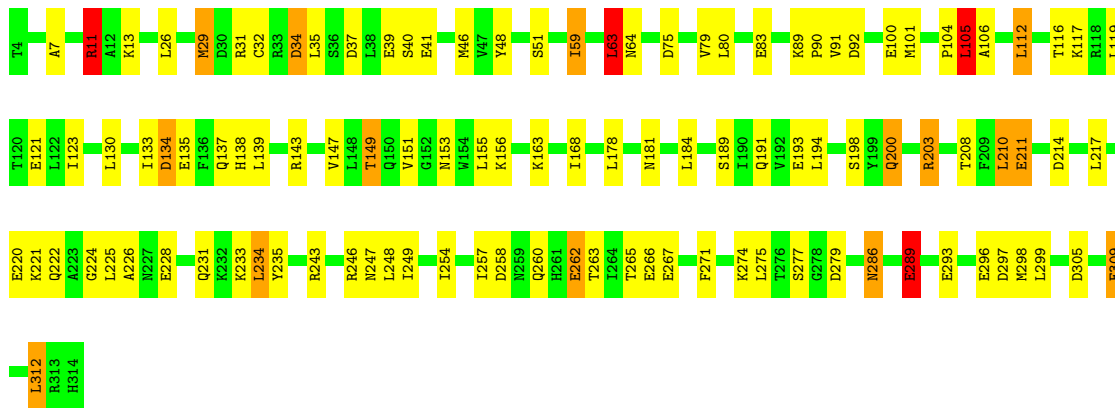




• Molecule 1: VchTnsC

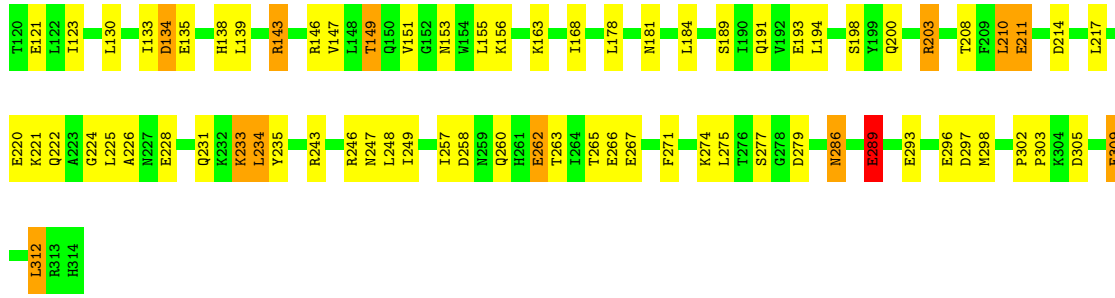


• Molecule 1: VchTnsC



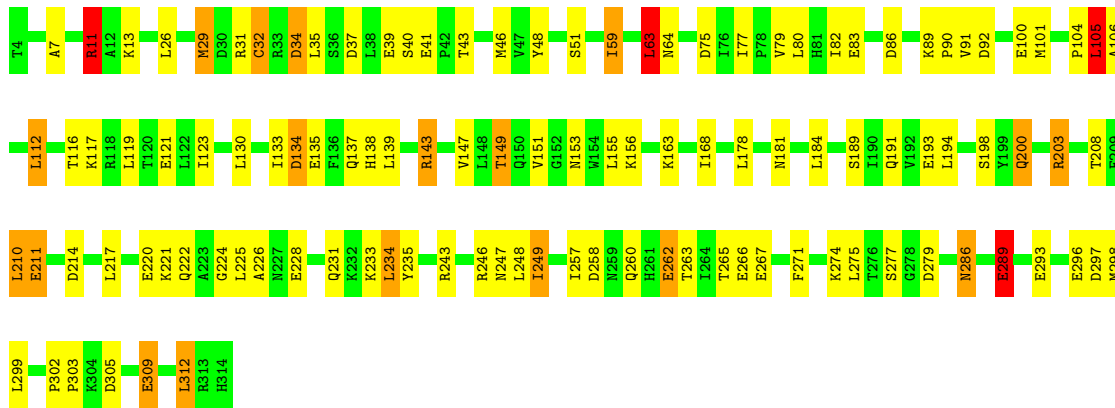
• Molecule 1: VchTnsC





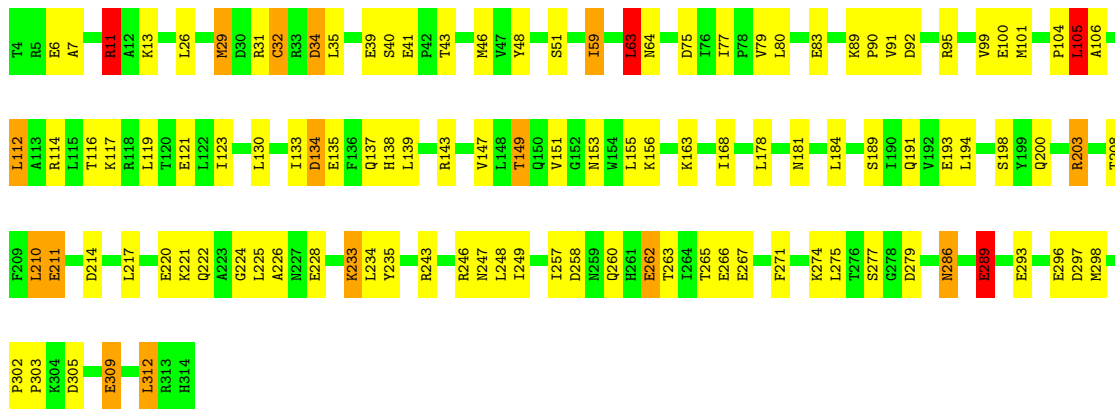
• Molecule 1: VchTnsC

Chain G: 63% 30% 6%



• Molecule 1: VchTnsC

Chain H: 64% 30% 5%



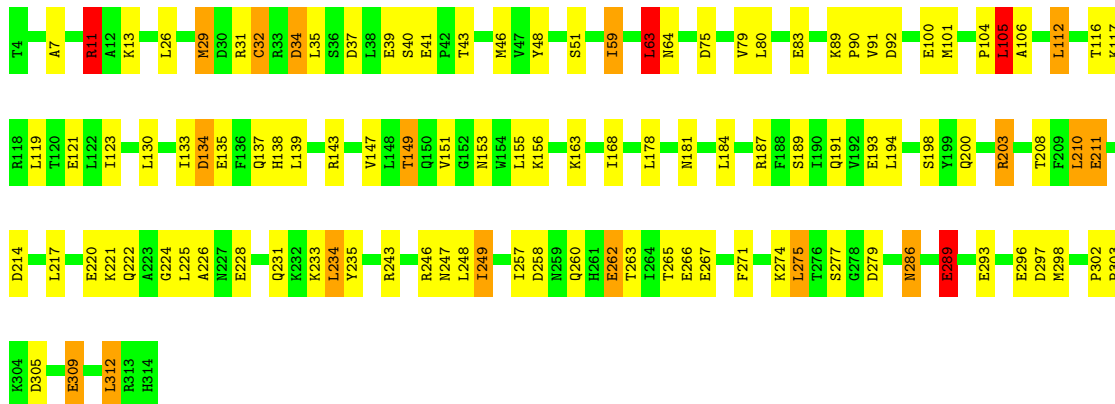
• Molecule 1: VchTnsC

Chain I: 63% 30% 5%

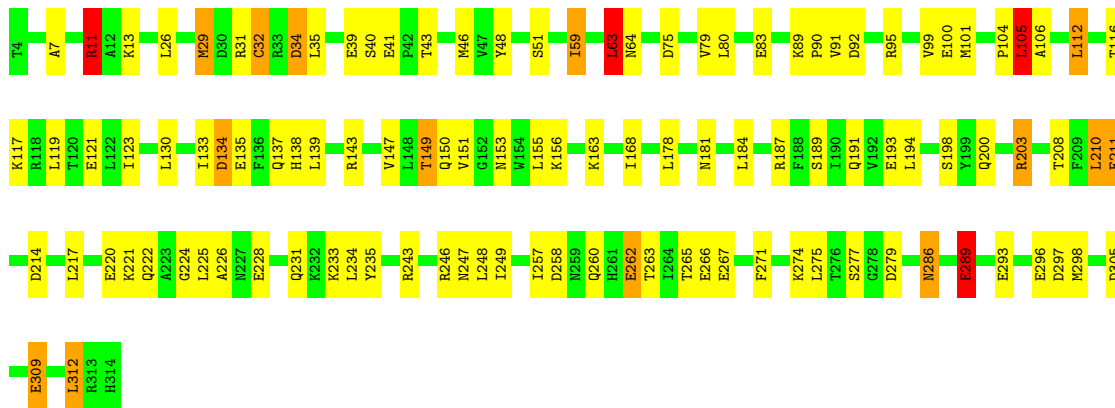




• Molecule 1: VchTnsC

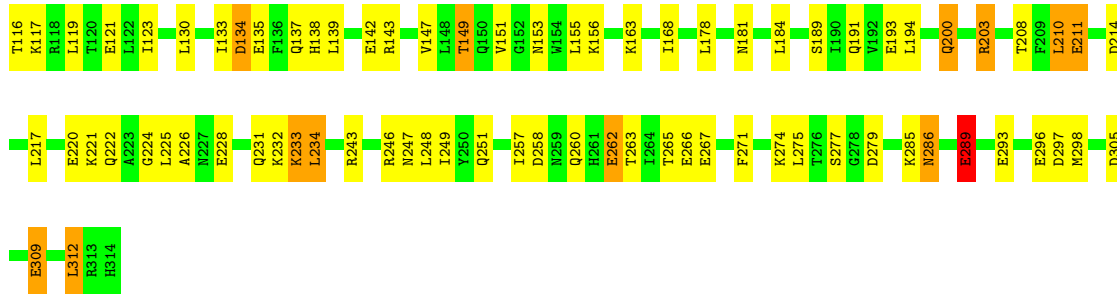


• Molecule 1: VchTnsC

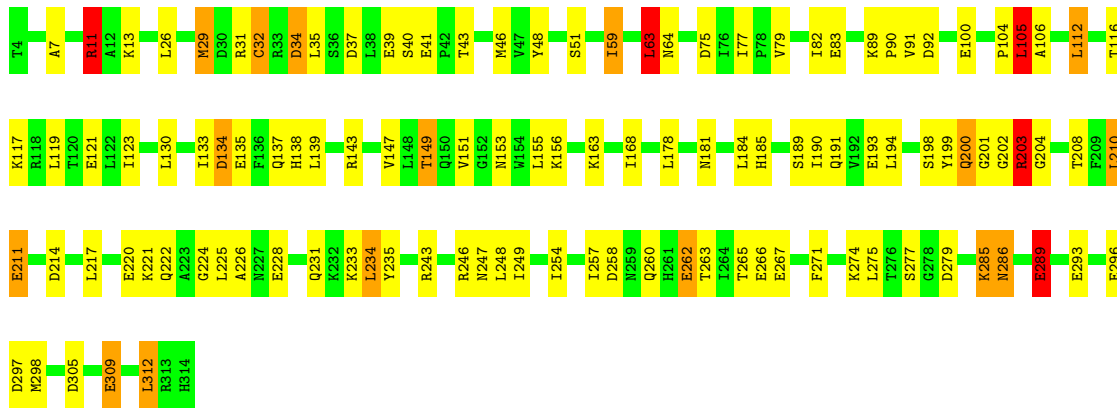


• Molecule 1: VchTnsC

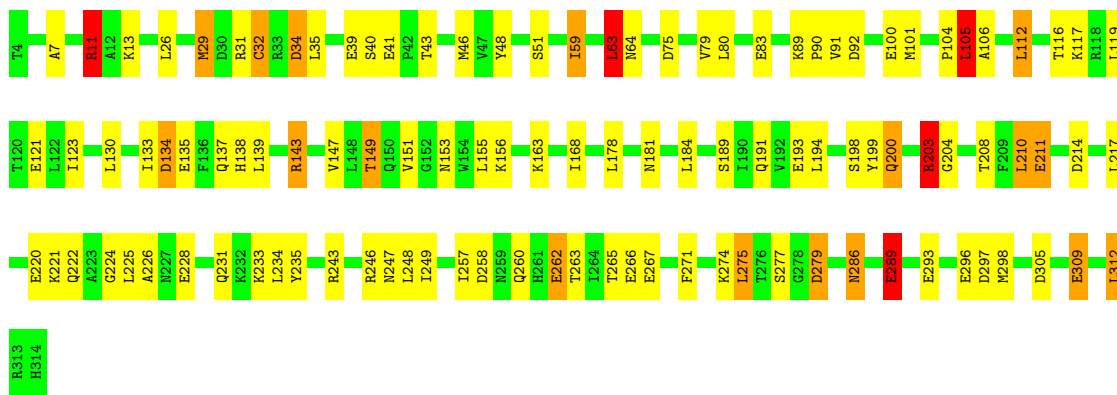




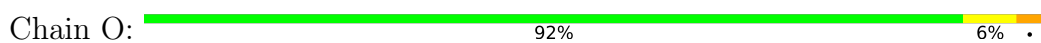
• Molecule 1: VchTnsC



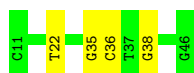
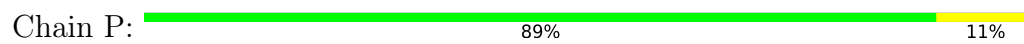
• Molecule 1: VchTnsC



• Molecule 2: DNA (36-MER)



• Molecule 3: DNA (36-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	125000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	A	0.43	0/2511	0.86	12/3395 (0.4%)
1	B	0.43	0/2511	0.86	12/3395 (0.4%)
1	C	0.43	0/2511	0.86	12/3395 (0.4%)
1	D	0.43	0/2511	0.86	12/3395 (0.4%)
1	E	0.43	0/2511	0.86	12/3395 (0.4%)
1	F	0.43	0/2511	0.86	12/3395 (0.4%)
1	G	0.43	0/2511	0.86	12/3395 (0.4%)
1	H	0.43	0/2511	0.86	12/3395 (0.4%)
1	I	0.43	0/2511	0.86	13/3395 (0.4%)
1	J	0.43	0/2511	0.86	12/3395 (0.4%)
1	K	0.43	0/2511	0.86	12/3395 (0.4%)
1	L	0.43	0/2511	0.86	12/3395 (0.4%)
1	M	0.43	0/2511	0.86	13/3395 (0.4%)
1	N	0.43	0/2511	0.86	12/3395 (0.4%)
2	O	0.77	0/827	1.03	3/1273 (0.2%)
3	P	0.75	0/825	0.99	0/1267
All	All	0.45	0/36806	0.87	173/50070 (0.3%)

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
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	1
1	I	0	1
1	J	0	1
1	K	0	1
1	L	0	1
1	M	0	1
1	N	0	1
All	All	0	14

There are no bond length outliers.

All (173) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	75	ASP	CB-CG-OD1	8.93	126.34	118.30
1	H	75	ASP	CB-CG-OD1	8.90	126.31	118.30
1	C	75	ASP	CB-CG-OD1	8.88	126.30	118.30
1	E	75	ASP	CB-CG-OD1	8.86	126.28	118.30
1	K	75	ASP	CB-CG-OD1	8.86	126.28	118.30
1	F	75	ASP	CB-CG-OD1	8.86	126.27	118.30
1	M	75	ASP	CB-CG-OD1	8.86	126.27	118.30
1	L	75	ASP	CB-CG-OD1	8.85	126.27	118.30
1	N	75	ASP	CB-CG-OD1	8.84	126.26	118.30
1	D	75	ASP	CB-CG-OD1	8.83	126.25	118.30
1	J	75	ASP	CB-CG-OD1	8.82	126.24	118.30
1	G	75	ASP	CB-CG-OD1	8.82	126.24	118.30
1	I	75	ASP	CB-CG-OD1	8.82	126.24	118.30
1	A	75	ASP	CB-CG-OD1	8.82	126.23	118.30
2	O	17	DT	OP2-P-O3'	8.16	123.15	105.20
2	O	18	DA	OP1-P-OP2	-7.96	107.66	119.60
1	H	11	ARG	CA-CB-CG	7.33	129.53	113.40
1	C	11	ARG	CA-CB-CG	7.32	129.50	113.40
1	M	11	ARG	CA-CB-CG	7.32	129.50	113.40
1	N	11	ARG	CA-CB-CG	7.32	129.49	113.40
1	D	11	ARG	CA-CB-CG	7.31	129.49	113.40
1	E	11	ARG	CA-CB-CG	7.31	129.49	113.40
1	G	11	ARG	CA-CB-CG	7.31	129.48	113.40
1	I	11	ARG	CA-CB-CG	7.31	129.48	113.40
1	K	11	ARG	CA-CB-CG	7.31	129.48	113.40
1	J	11	ARG	CA-CB-CG	7.31	129.48	113.40
1	A	11	ARG	CA-CB-CG	7.30	129.46	113.40
1	B	11	ARG	CA-CB-CG	7.30	129.46	113.40
1	F	11	ARG	CA-CB-CG	7.30	129.46	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	11	ARG	CA-CB-CG	7.30	129.46	113.40
1	A	105	LEU	CA-CB-CG	7.26	132.01	115.30
1	E	105	LEU	CA-CB-CG	7.25	131.98	115.30
1	H	105	LEU	CA-CB-CG	7.25	131.98	115.30
1	L	105	LEU	CA-CB-CG	7.25	131.97	115.30
1	M	105	LEU	CA-CB-CG	7.25	131.96	115.30
1	D	105	LEU	CA-CB-CG	7.24	131.96	115.30
1	B	105	LEU	CA-CB-CG	7.24	131.94	115.30
1	C	105	LEU	CA-CB-CG	7.24	131.94	115.30
1	J	105	LEU	CA-CB-CG	7.24	131.94	115.30
1	F	105	LEU	CA-CB-CG	7.23	131.94	115.30
1	N	105	LEU	CA-CB-CG	7.23	131.93	115.30
1	K	105	LEU	CA-CB-CG	7.23	131.93	115.30
1	I	105	LEU	CA-CB-CG	7.23	131.93	115.30
1	G	105	LEU	CA-CB-CG	7.23	131.92	115.30
1	K	112	LEU	CA-CB-CG	6.91	131.19	115.30
1	B	112	LEU	CA-CB-CG	6.91	131.18	115.30
1	I	112	LEU	CA-CB-CG	6.91	131.18	115.30
1	A	112	LEU	CA-CB-CG	6.90	131.18	115.30
1	C	112	LEU	CA-CB-CG	6.90	131.17	115.30
1	J	112	LEU	CA-CB-CG	6.90	131.17	115.30
1	N	112	LEU	CA-CB-CG	6.90	131.17	115.30
1	D	112	LEU	CA-CB-CG	6.89	131.15	115.30
1	H	112	LEU	CA-CB-CG	6.89	131.15	115.30
1	E	112	LEU	CA-CB-CG	6.88	131.13	115.30
1	F	112	LEU	CA-CB-CG	6.88	131.13	115.30
1	L	112	LEU	CA-CB-CG	6.88	131.13	115.30
1	G	112	LEU	CA-CB-CG	6.88	131.13	115.30
1	M	112	LEU	CA-CB-CG	6.88	131.13	115.30
1	A	289	GLU	CA-CB-CG	6.59	127.89	113.40
1	F	289	GLU	CA-CB-CG	6.59	127.89	113.40
1	B	289	GLU	CA-CB-CG	6.58	127.89	113.40
1	G	289	GLU	CA-CB-CG	6.58	127.88	113.40
1	J	309	GLU	CA-CB-CG	6.58	127.88	113.40
1	L	289	GLU	CA-CB-CG	6.58	127.87	113.40
1	L	309	GLU	CA-CB-CG	6.58	127.87	113.40
1	M	289	GLU	CA-CB-CG	6.58	127.87	113.40
1	A	309	GLU	CA-CB-CG	6.57	127.86	113.40
1	K	289	GLU	CA-CB-CG	6.57	127.86	113.40
1	C	289	GLU	CA-CB-CG	6.57	127.86	113.40
1	H	289	GLU	CA-CB-CG	6.57	127.86	113.40
1	H	309	GLU	CA-CB-CG	6.57	127.85	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	289	GLU	CA-CB-CG	6.57	127.84	113.40
1	I	289	GLU	CA-CB-CG	6.57	127.84	113.40
1	I	309	GLU	CA-CB-CG	6.57	127.84	113.40
1	K	309	GLU	CA-CB-CG	6.56	127.84	113.40
1	C	309	GLU	CA-CB-CG	6.56	127.83	113.40
1	J	289	GLU	CA-CB-CG	6.56	127.83	113.40
1	N	289	GLU	CA-CB-CG	6.56	127.83	113.40
1	M	309	GLU	CA-CB-CG	6.56	127.83	113.40
1	E	289	GLU	CA-CB-CG	6.55	127.82	113.40
1	G	309	GLU	CA-CB-CG	6.55	127.82	113.40
1	B	309	GLU	CA-CB-CG	6.55	127.82	113.40
1	F	309	GLU	CA-CB-CG	6.55	127.81	113.40
1	D	309	GLU	CA-CB-CG	6.55	127.81	113.40
1	E	309	GLU	CA-CB-CG	6.55	127.80	113.40
1	N	309	GLU	CA-CB-CG	6.54	127.80	113.40
1	J	203	ARG	CB-CG-CD	6.11	127.50	111.60
1	F	203	ARG	CB-CG-CD	6.11	127.49	111.60
1	D	203	ARG	CB-CG-CD	6.11	127.48	111.60
1	K	203	ARG	CB-CG-CD	6.11	127.48	111.60
1	E	203	ARG	CB-CG-CD	6.11	127.48	111.60
1	L	203	ARG	CB-CG-CD	6.10	127.46	111.60
1	G	203	ARG	CB-CG-CD	6.10	127.46	111.60
1	M	203	ARG	CB-CG-CD	6.10	127.46	111.60
1	N	203	ARG	CB-CG-CD	6.10	127.46	111.60
1	B	203	ARG	CB-CG-CD	6.09	127.43	111.60
1	H	203	ARG	CB-CG-CD	6.08	127.42	111.60
1	C	203	ARG	CB-CG-CD	6.08	127.42	111.60
1	I	203	ARG	CB-CG-CD	6.08	127.42	111.60
1	A	203	ARG	CB-CG-CD	6.08	127.41	111.60
1	G	312	LEU	CA-CB-CG	5.67	128.34	115.30
1	E	312	LEU	CA-CB-CG	5.66	128.32	115.30
1	L	312	LEU	CA-CB-CG	5.66	128.32	115.30
1	D	312	LEU	CA-CB-CG	5.66	128.31	115.30
1	J	312	LEU	CA-CB-CG	5.66	128.31	115.30
1	M	312	LEU	CA-CB-CG	5.66	128.31	115.30
1	A	312	LEU	CA-CB-CG	5.65	128.30	115.30
1	B	312	LEU	CA-CB-CG	5.65	128.30	115.30
1	H	312	LEU	CA-CB-CG	5.65	128.31	115.30
1	C	312	LEU	CA-CB-CG	5.65	128.29	115.30
1	I	312	LEU	CA-CB-CG	5.65	128.30	115.30
1	F	312	LEU	CA-CB-CG	5.65	128.29	115.30
1	K	312	LEU	CA-CB-CG	5.65	128.29	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	312	LEU	CA-CB-CG	5.65	128.29	115.30
1	C	63	LEU	CA-CB-CG	5.50	127.94	115.30
1	D	63	LEU	CA-CB-CG	5.49	127.93	115.30
1	E	63	LEU	CA-CB-CG	5.48	127.91	115.30
1	L	63	LEU	CA-CB-CG	5.48	127.90	115.30
1	A	63	LEU	CA-CB-CG	5.47	127.89	115.30
1	B	63	LEU	CA-CB-CG	5.47	127.89	115.30
1	G	63	LEU	CA-CB-CG	5.47	127.89	115.30
1	H	63	LEU	CA-CB-CG	5.47	127.89	115.30
1	N	63	LEU	CA-CB-CG	5.47	127.89	115.30
1	J	63	LEU	CA-CB-CG	5.47	127.88	115.30
1	K	63	LEU	CA-CB-CG	5.47	127.88	115.30
1	F	63	LEU	CA-CB-CG	5.46	127.87	115.30
1	I	63	LEU	CA-CB-CG	5.46	127.87	115.30
1	M	63	LEU	CA-CB-CG	5.46	127.87	115.30
2	O	17	DT	O4'-C1'-N1	5.41	111.79	108.00
1	H	225	LEU	CA-CB-CG	5.20	127.25	115.30
1	K	225	LEU	CA-CB-CG	5.20	127.25	115.30
1	G	225	LEU	CA-CB-CG	5.19	127.24	115.30
1	C	225	LEU	CA-CB-CG	5.19	127.24	115.30
1	A	225	LEU	CA-CB-CG	5.19	127.23	115.30
1	D	225	LEU	CA-CB-CG	5.19	127.23	115.30
1	N	225	LEU	CA-CB-CG	5.19	127.23	115.30
1	M	225	LEU	CA-CB-CG	5.19	127.23	115.30
1	J	225	LEU	CA-CB-CG	5.18	127.22	115.30
1	I	225	LEU	CA-CB-CG	5.18	127.22	115.30
1	L	225	LEU	CA-CB-CG	5.18	127.21	115.30
1	E	225	LEU	CA-CB-CG	5.18	127.21	115.30
1	F	225	LEU	CA-CB-CG	5.17	127.19	115.30
1	B	225	LEU	CA-CB-CG	5.16	127.18	115.30
1	A	203	ARG	CG-CD-NE	5.11	122.52	111.80
1	I	203	ARG	CG-CD-NE	5.10	122.50	111.80
1	G	203	ARG	CG-CD-NE	5.09	122.50	111.80
1	B	203	ARG	CG-CD-NE	5.09	122.49	111.80
1	D	203	ARG	CG-CD-NE	5.09	122.49	111.80
1	C	203	ARG	CG-CD-NE	5.09	122.48	111.80
1	L	203	ARG	CG-CD-NE	5.09	122.48	111.80
1	K	203	ARG	CG-CD-NE	5.08	122.47	111.80
1	E	203	ARG	CG-CD-NE	5.08	122.47	111.80
1	J	203	ARG	CG-CD-NE	5.08	122.47	111.80
1	F	203	ARG	CG-CD-NE	5.08	122.47	111.80
1	M	203	ARG	CG-CD-NE	5.08	122.46	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	203	ARG	CG-CD-NE	5.07	122.45	111.80
1	N	203	ARG	CG-CD-NE	5.07	122.45	111.80
1	L	262	GLU	CA-CB-CG	5.07	124.56	113.40
1	E	262	GLU	CA-CB-CG	5.06	124.54	113.40
1	H	262	GLU	CA-CB-CG	5.06	124.54	113.40
1	J	262	GLU	CA-CB-CG	5.06	124.54	113.40
1	F	262	GLU	CA-CB-CG	5.06	124.54	113.40
1	N	262	GLU	CA-CB-CG	5.06	124.54	113.40
1	C	262	GLU	CA-CB-CG	5.06	124.53	113.40
1	I	262	GLU	CA-CB-CG	5.06	124.53	113.40
1	M	262	GLU	CA-CB-CG	5.05	124.52	113.40
1	A	262	GLU	CA-CB-CG	5.05	124.51	113.40
1	B	262	GLU	CA-CB-CG	5.05	124.51	113.40
1	D	262	GLU	CA-CB-CG	5.05	124.51	113.40
1	K	262	GLU	CA-CB-CG	5.05	124.51	113.40
1	G	262	GLU	CA-CB-CG	5.04	124.50	113.40
1	I	285	LYS	C-N-CA	5.02	134.24	121.70
1	M	285	LYS	C-N-CA	5.01	134.23	121.70

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	LEU	Peptide
1	B	105	LEU	Peptide
1	C	105	LEU	Peptide
1	D	105	LEU	Peptide
1	E	105	LEU	Peptide
1	F	105	LEU	Peptide
1	G	105	LEU	Peptide
1	H	105	LEU	Peptide
1	I	105	LEU	Peptide
1	J	105	LEU	Peptide
1	K	105	LEU	Peptide
1	L	105	LEU	Peptide
1	M	105	LEU	Peptide
1	N	105	LEU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2463	0	2497	42	0
1	B	2463	0	2497	43	0
1	C	2463	0	2495	38	0
1	D	2463	0	2497	43	0
1	E	2463	0	2497	40	0
1	F	2463	0	2497	39	0
1	G	2463	0	2497	47	0
1	H	2463	0	2495	49	0
1	I	2463	0	2497	48	0
1	J	2463	0	2497	43	0
1	K	2463	0	2497	43	0
1	L	2463	0	2497	48	0
1	M	2463	0	2497	58	0
1	N	2463	0	2497	57	0
2	O	737	0	404	5	0
3	P	739	0	410	3	0
4	A	31	0	12	0	0
4	B	31	0	12	0	0
4	C	31	0	12	0	0
4	D	31	0	12	1	0
4	E	31	0	12	0	0
4	F	31	0	12	0	0
4	G	31	0	12	0	0
4	H	31	0	12	0	0
4	I	31	0	12	0	0
4	J	31	0	12	0	0
4	K	31	0	12	1	0
4	L	31	0	12	2	0
4	M	31	0	12	0	0
4	N	31	0	12	0	0
All	All	36392	0	35936	625	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 9.

All (625) 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)
1:B:200:GLN:NE2	1:B:299:LEU:HD13	1.37	1.39
1:M:199:TYR:OH	1:M:204:GLY:N	1.66	1.29
1:I:200:GLN:HG3	1:I:299:LEU:HD13	1.22	1.19
1:N:199:TYR:OH	1:N:204:GLY:CA	1.92	1.17
1:N:200:GLN:OE1	1:N:231:GLN:C	1.86	1.14
1:L:200:GLN:HE21	1:L:231:GLN:C	1.55	1.09
1:N:199:TYR:OH	1:N:204:GLY:N	1.86	1.08
1:H:200:GLN:CD	1:H:235:TYR:HB2	1.73	1.07
1:E:200:GLN:HG2	1:E:299:LEU:HB3	1.36	1.07
1:B:200:GLN:NE2	1:B:299:LEU:CD1	2.18	1.04
1:A:200:GLN:NE2	1:A:231:GLN:HB2	1.74	1.03
1:N:199:TYR:OH	1:N:204:GLY:HA2	1.56	1.01
1:M:199:TYR:HE2	1:M:202:GLY:N	1.60	0.98
1:I:200:GLN:NE2	1:I:299:LEU:HB2	1.81	0.95
1:L:200:GLN:NE2	1:L:232:LYS:N	2.15	0.93
1:M:199:TYR:OH	1:M:203:ARG:C	2.06	0.93
1:N:200:GLN:OE1	1:N:231:GLN:O	1.86	0.93
1:B:200:GLN:HE21	1:B:299:LEU:HD13	1.24	0.91
1:H:200:GLN:CD	1:H:235:TYR:CB	2.25	0.91
1:N:199:TYR:OH	1:N:203:ARG:C	2.08	0.91
1:L:200:GLN:NE2	1:L:231:GLN:C	2.25	0.90
1:I:200:GLN:HG3	1:I:299:LEU:CD1	2.02	0.89
1:D:200:GLN:O	1:D:200:GLN:NE2	2.08	0.87
1:M:200:GLN:O	1:M:200:GLN:NE2	2.08	0.86
1:N:200:GLN:OE1	1:N:231:GLN:HB2	1.77	0.84
1:M:199:TYR:OH	1:M:204:GLY:CA	2.26	0.83
1:H:200:GLN:CG	1:H:235:TYR:CG	2.56	0.83
1:D:200:GLN:HG2	1:D:299:LEU:HD13	1.59	0.82
1:L:200:GLN:NE2	1:L:232:LYS:HA	1.96	0.80
1:L:200:GLN:NE2	1:L:232:LYS:CA	2.45	0.78
1:K:200:GLN:NE2	1:K:231:GLN:HB2	1.99	0.78
1:J:200:GLN:NE2	1:J:231:GLN:HB2	1.99	0.77
1:A:200:GLN:HE21	1:A:231:GLN:HB2	1.49	0.77
1:N:200:GLN:OE1	1:N:231:GLN:CB	2.33	0.76
1:E:200:GLN:O	1:E:200:GLN:NE2	2.18	0.76
1:N:199:TYR:CZ	1:N:204:GLY:CA	2.69	0.75
1:I:200:GLN:CD	1:I:299:LEU:HB3	2.08	0.74
1:B:200:GLN:HE22	1:B:299:LEU:CD1	2.00	0.73
1:E:200:GLN:CG	1:E:299:LEU:HB3	2.18	0.72
1:G:200:GLN:CD	1:G:299:LEU:HD13	2.09	0.72
1:K:200:GLN:HE22	1:K:231:GLN:HB2	1.55	0.71
1:H:6:GLU:HG3	1:N:31:ARG:HH22	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:200:GLN:HE22	1:J:231:GLN:HB2	1.55	0.70
1:L:200:GLN:HE22	1:L:232:LYS:N	1.85	0.70
1:I:200:GLN:CD	1:I:299:LEU:CB	2.59	0.70
1:B:31:ARG:O	1:B:35:LEU:HB2	1.92	0.69
1:A:31:ARG:O	1:A:35:LEU:HB2	1.93	0.69
1:H:31:ARG:O	1:H:35:LEU:HB2	1.92	0.69
1:K:7:ALA:O	1:K:11:ARG:HB3	1.93	0.69
1:C:7:ALA:O	1:C:11:ARG:HB3	1.93	0.69
1:E:7:ALA:O	1:E:11:ARG:HB3	1.93	0.69
1:I:7:ALA:O	1:I:11:ARG:HB3	1.93	0.69
1:B:7:ALA:O	1:B:11:ARG:HB3	1.93	0.69
1:D:7:ALA:O	1:D:11:ARG:HB3	1.93	0.69
1:L:31:ARG:O	1:L:35:LEU:HB2	1.92	0.69
1:D:31:ARG:O	1:D:35:LEU:HB2	1.93	0.69
1:I:31:ARG:O	1:I:35:LEU:HB2	1.93	0.69
1:G:31:ARG:O	1:G:35:LEU:HB2	1.92	0.69
1:J:31:ARG:O	1:J:35:LEU:HB2	1.92	0.69
1:M:199:TYR:HH	1:M:203:ARG:C	1.94	0.69
1:N:7:ALA:O	1:N:11:ARG:HB3	1.93	0.69
1:G:7:ALA:O	1:G:11:ARG:HB3	1.93	0.69
1:H:7:ALA:O	1:H:11:ARG:HB3	1.93	0.69
1:J:200:GLN:OE1	1:J:235:TYR:HB2	1.93	0.69
1:A:7:ALA:O	1:A:11:ARG:HB3	1.93	0.68
1:E:31:ARG:O	1:E:35:LEU:HB2	1.92	0.68
1:M:31:ARG:O	1:M:35:LEU:HB2	1.93	0.68
1:C:31:ARG:O	1:C:35:LEU:HB2	1.93	0.68
1:D:104:PRO:HB2	1:D:106:ALA:HB2	1.76	0.68
1:J:7:ALA:O	1:J:11:ARG:HB3	1.93	0.68
1:K:200:GLN:OE1	1:K:235:TYR:HB2	1.93	0.68
1:M:7:ALA:O	1:M:11:ARG:HB3	1.93	0.68
1:N:31:ARG:O	1:N:35:LEU:HB2	1.92	0.68
1:A:104:PRO:HB2	1:A:106:ALA:HB2	1.76	0.68
1:H:200:GLN:HG2	1:H:235:TYR:CG	2.29	0.68
1:H:200:GLN:HG2	1:H:235:TYR:CD1	2.28	0.68
1:I:104:PRO:HB2	1:I:106:ALA:HB2	1.76	0.68
1:F:31:ARG:O	1:F:35:LEU:HB2	1.92	0.68
1:L:104:PRO:HB2	1:L:106:ALA:HB2	1.76	0.68
1:B:104:PRO:HB2	1:B:106:ALA:HB2	1.76	0.68
1:L:7:ALA:O	1:L:11:ARG:HB3	1.93	0.68
1:G:104:PRO:HB2	1:G:106:ALA:HB2	1.76	0.67
1:H:104:PRO:HB2	1:H:106:ALA:HB2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:31:ARG:O	1:K:35:LEU:HB2	1.93	0.67
1:K:104:PRO:HB2	1:K:106:ALA:HB2	1.76	0.67
1:N:104:PRO:HB2	1:N:106:ALA:HB2	1.76	0.67
1:F:7:ALA:O	1:F:11:ARG:HB3	1.93	0.67
1:F:104:PRO:HB2	1:F:106:ALA:HB2	1.76	0.67
1:J:104:PRO:HB2	1:J:106:ALA:HB2	1.76	0.67
1:M:104:PRO:HB2	1:M:106:ALA:HB2	1.76	0.66
1:C:104:PRO:HB2	1:C:106:ALA:HB2	1.76	0.66
1:E:104:PRO:HB2	1:E:106:ALA:HB2	1.76	0.66
1:E:200:GLN:C	1:E:200:GLN:HE21	1.99	0.66
1:J:200:GLN:HE22	1:J:231:GLN:CB	2.09	0.66
1:F:89:LYS:HE3	1:F:90:PRO:HD2	1.79	0.65
1:N:89:LYS:HE3	1:N:90:PRO:HD2	1.79	0.65
1:E:89:LYS:HE3	1:E:90:PRO:HD2	1.79	0.65
1:B:89:LYS:HE3	1:B:90:PRO:HD2	1.79	0.65
1:K:200:GLN:HE22	1:K:231:GLN:CB	2.09	0.65
1:E:200:GLN:HG2	1:E:299:LEU:CB	2.21	0.64
1:I:89:LYS:HE3	1:I:90:PRO:HD2	1.79	0.64
1:J:89:LYS:HE3	1:J:90:PRO:HD2	1.79	0.64
1:G:89:LYS:HE3	1:G:90:PRO:HD2	1.79	0.64
1:M:89:LYS:HE3	1:M:90:PRO:HD2	1.79	0.64
1:L:89:LYS:HE3	1:L:90:PRO:HD2	1.79	0.64
1:H:89:LYS:HE3	1:H:90:PRO:HD2	1.79	0.63
1:A:89:LYS:HE3	1:A:90:PRO:HD2	1.79	0.63
1:I:200:GLN:NE2	1:I:299:LEU:CB	2.59	0.63
1:D:89:LYS:HE3	1:D:90:PRO:HD2	1.79	0.63
1:C:134:ASP:HB3	1:C:135:GLU:HG2	1.82	0.62
1:F:222:GLN:HG3	1:F:224:GLY:H	1.64	0.62
1:K:134:ASP:HB3	1:K:135:GLU:HG2	1.82	0.62
1:C:89:LYS:HE3	1:C:90:PRO:HD2	1.79	0.62
1:K:89:LYS:HE3	1:K:90:PRO:HD2	1.79	0.62
1:L:134:ASP:HB3	1:L:135:GLU:HG2	1.82	0.62
1:L:222:GLN:HG3	1:L:224:GLY:H	1.64	0.62
1:H:134:ASP:HB3	1:H:135:GLU:HG2	1.82	0.62
1:N:222:GLN:HG3	1:N:224:GLY:H	1.64	0.62
1:F:134:ASP:HB3	1:F:135:GLU:HG2	1.82	0.62
1:A:134:ASP:HB3	1:A:135:GLU:HG2	1.81	0.62
1:B:134:ASP:HB3	1:B:135:GLU:HG2	1.82	0.62
1:D:222:GLN:HG3	1:D:224:GLY:H	1.64	0.62
1:E:134:ASP:HB3	1:E:135:GLU:HG2	1.82	0.62
1:M:222:GLN:HG3	1:M:224:GLY:H	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:222:GLN:HG3	1:I:224:GLY:H	1.64	0.61
1:K:187:ARG:NH1	4:L:401:ATP:O3G	2.31	0.61
1:C:222:GLN:HG3	1:C:224:GLY:H	1.64	0.61
1:F:181:ASN:HB3	1:F:184:LEU:HB2	1.82	0.61
1:N:134:ASP:HB3	1:N:135:GLU:HG2	1.82	0.61
1:J:222:GLN:HG3	1:J:224:GLY:H	1.64	0.61
1:D:134:ASP:HB3	1:D:135:GLU:HG2	1.82	0.61
1:E:222:GLN:HG3	1:E:224:GLY:H	1.64	0.61
1:G:134:ASP:HB3	1:G:135:GLU:HG2	1.82	0.61
1:J:134:ASP:HB3	1:J:135:GLU:HG2	1.82	0.61
1:H:222:GLN:HG3	1:H:224:GLY:H	1.64	0.61
1:A:222:GLN:HG3	1:A:224:GLY:H	1.64	0.61
1:M:134:ASP:HB3	1:M:135:GLU:HG2	1.82	0.61
1:A:46:MET:HB3	1:A:191:GLN:HG3	1.83	0.61
1:J:46:MET:HB3	1:J:191:GLN:HG3	1.83	0.61
1:E:181:ASN:HB3	1:E:184:LEU:HB2	1.83	0.61
1:N:200:GLN:HE21	1:N:200:GLN:HA	1.66	0.61
1:B:222:GLN:HG3	1:B:224:GLY:H	1.64	0.61
1:G:222:GLN:HG3	1:G:224:GLY:H	1.64	0.61
1:I:46:MET:HB3	1:I:191:GLN:HG3	1.83	0.61
1:K:222:GLN:HG3	1:K:224:GLY:H	1.64	0.61
1:C:181:ASN:HB3	1:C:184:LEU:HB2	1.82	0.60
1:G:46:MET:HB3	1:G:191:GLN:HG3	1.83	0.60
1:H:46:MET:HB3	1:H:191:GLN:HG3	1.83	0.60
1:I:134:ASP:HB3	1:I:135:GLU:HG2	1.82	0.60
1:K:46:MET:HB3	1:K:191:GLN:HG3	1.83	0.60
1:M:181:ASN:HB3	1:M:184:LEU:HB2	1.82	0.60
1:A:289:GLU:N	1:A:289:GLU:OE1	2.35	0.60
1:B:46:MET:HB3	1:B:191:GLN:HG3	1.83	0.60
1:B:181:ASN:HB3	1:B:184:LEU:HB2	1.83	0.60
1:E:289:GLU:OE1	1:E:289:GLU:N	2.35	0.60
1:G:181:ASN:HB3	1:G:184:LEU:HB2	1.82	0.60
1:H:181:ASN:HB3	1:H:184:LEU:HB2	1.82	0.60
1:H:200:GLN:CG	1:H:235:TYR:CB	2.78	0.60
1:H:289:GLU:N	1:H:289:GLU:OE1	2.35	0.60
1:K:289:GLU:N	1:K:289:GLU:OE1	2.35	0.60
1:D:46:MET:HB3	1:D:191:GLN:HG3	1.83	0.60
1:J:181:ASN:HB3	1:J:184:LEU:HB2	1.82	0.60
1:L:46:MET:HB3	1:L:191:GLN:HG3	1.83	0.60
1:L:200:GLN:HE22	1:L:232:LYS:CA	2.12	0.60
1:I:289:GLU:N	1:I:289:GLU:OE1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:181:ASN:HB3	1:K:184:LEU:HB2	1.82	0.60
1:A:181:ASN:HB3	1:A:184:LEU:HB2	1.82	0.60
1:D:289:GLU:N	1:D:289:GLU:OE1	2.35	0.60
1:L:181:ASN:HB3	1:L:184:LEU:HB2	1.82	0.60
1:J:289:GLU:OE1	1:J:289:GLU:N	2.35	0.60
1:D:181:ASN:HB3	1:D:184:LEU:HB2	1.82	0.59
1:E:46:MET:HB3	1:E:191:GLN:HG3	1.83	0.59
1:I:181:ASN:HB3	1:I:184:LEU:HB2	1.82	0.59
1:M:289:GLU:N	1:M:289:GLU:OE1	2.35	0.59
1:N:199:TYR:OH	1:N:203:ARG:O	2.19	0.59
1:C:289:GLU:N	1:C:289:GLU:OE1	2.35	0.59
1:F:34:ASP:OD1	1:F:34:ASP:N	2.36	0.59
1:G:289:GLU:N	1:G:289:GLU:OE1	2.35	0.59
1:L:289:GLU:OE1	1:L:289:GLU:N	2.35	0.59
1:M:46:MET:HB3	1:M:191:GLN:HG3	1.83	0.59
1:N:181:ASN:HB3	1:N:184:LEU:HB2	1.82	0.59
1:I:34:ASP:OD1	1:I:34:ASP:N	2.35	0.59
1:B:34:ASP:OD1	1:B:34:ASP:N	2.35	0.59
1:N:46:MET:HB3	1:N:191:GLN:HG3	1.83	0.59
1:N:89:LYS:HB2	1:N:92:ASP:HB2	1.85	0.59
1:N:289:GLU:N	1:N:289:GLU:OE1	2.35	0.59
1:A:89:LYS:HB2	1:A:92:ASP:HB2	1.85	0.59
1:C:46:MET:HB3	1:C:191:GLN:HG3	1.83	0.59
1:F:289:GLU:N	1:F:289:GLU:OE1	2.35	0.59
1:B:89:LYS:HB2	1:B:92:ASP:HB2	1.85	0.59
1:B:289:GLU:N	1:B:289:GLU:OE1	2.35	0.59
1:F:46:MET:HB3	1:F:191:GLN:HG3	1.83	0.59
1:J:34:ASP:N	1:J:34:ASP:OD1	2.35	0.59
1:D:34:ASP:OD1	1:D:34:ASP:N	2.35	0.59
1:F:89:LYS:HB2	1:F:92:ASP:HB2	1.85	0.59
1:H:89:LYS:HB2	1:H:92:ASP:HB2	1.85	0.59
1:D:13:LYS:O	1:D:246:ARG:NH2	2.36	0.59
1:E:89:LYS:HB2	1:E:92:ASP:HB2	1.85	0.59
1:G:34:ASP:OD1	1:G:34:ASP:N	2.35	0.59
1:H:34:ASP:N	1:H:34:ASP:OD1	2.35	0.59
1:I:89:LYS:HB2	1:I:92:ASP:HB2	1.85	0.59
1:J:89:LYS:HB2	1:J:92:ASP:HB2	1.85	0.59
1:F:13:LYS:O	1:F:246:ARG:NH2	2.36	0.58
1:L:13:LYS:O	1:L:246:ARG:NH2	2.36	0.58
1:M:13:LYS:O	1:M:246:ARG:NH2	2.36	0.58
1:C:89:LYS:HB2	1:C:92:ASP:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:286:ASN:ND2	1:D:289:GLU:OE2	2.37	0.58
1:E:13:LYS:O	1:E:246:ARG:NH2	2.36	0.58
1:K:13:LYS:O	1:K:246:ARG:NH2	2.36	0.58
1:K:89:LYS:HB2	1:K:92:ASP:HB2	1.85	0.58
1:N:199:TYR:CZ	1:N:204:GLY:HA2	2.36	0.58
1:H:13:LYS:O	1:H:246:ARG:NH2	2.36	0.58
1:J:13:LYS:O	1:J:246:ARG:NH2	2.36	0.58
1:M:89:LYS:HB2	1:M:92:ASP:HB2	1.85	0.58
1:C:34:ASP:N	1:C:34:ASP:OD1	2.35	0.58
1:I:286:ASN:ND2	1:I:289:GLU:OE2	2.37	0.58
1:L:286:ASN:ND2	1:L:289:GLU:OE2	2.37	0.58
1:N:13:LYS:O	1:N:246:ARG:NH2	2.36	0.58
1:N:34:ASP:OD1	1:N:34:ASP:N	2.35	0.58
1:A:13:LYS:O	1:A:246:ARG:NH2	2.36	0.58
1:G:13:LYS:O	1:G:246:ARG:NH2	2.36	0.58
1:B:286:ASN:ND2	1:B:289:GLU:OE2	2.37	0.58
1:M:34:ASP:OD1	1:M:34:ASP:N	2.35	0.58
1:A:34:ASP:OD1	1:A:34:ASP:N	2.36	0.58
1:D:89:LYS:HB2	1:D:92:ASP:HB2	1.85	0.58
1:G:286:ASN:ND2	1:G:289:GLU:OE2	2.37	0.58
1:H:200:GLN:CG	1:H:235:TYR:CD1	2.84	0.58
1:L:89:LYS:HB2	1:L:92:ASP:HB2	1.85	0.58
1:B:13:LYS:O	1:B:246:ARG:NH2	2.36	0.58
1:C:13:LYS:O	1:C:246:ARG:NH2	2.36	0.58
1:E:34:ASP:N	1:E:34:ASP:OD1	2.35	0.57
1:I:13:LYS:O	1:I:246:ARG:NH2	2.36	0.57
1:L:34:ASP:N	1:L:34:ASP:OD1	2.36	0.57
1:G:89:LYS:HB2	1:G:92:ASP:HB2	1.85	0.57
1:C:79:VAL:HG23	1:C:130:LEU:HB3	1.87	0.57
1:F:79:VAL:HG23	1:F:130:LEU:HB3	1.87	0.57
1:K:79:VAL:HG23	1:K:130:LEU:HB3	1.87	0.57
1:M:32:CYS:SG	1:M:43:THR:OG1	2.55	0.57
1:A:286:ASN:ND2	1:A:289:GLU:OE2	2.37	0.57
1:H:79:VAL:HG23	1:H:130:LEU:HB3	1.87	0.57
1:C:286:ASN:ND2	1:C:289:GLU:OE2	2.37	0.57
1:K:286:ASN:ND2	1:K:289:GLU:OE2	2.37	0.57
1:N:286:ASN:ND2	1:N:289:GLU:OE2	2.37	0.57
1:K:34:ASP:OD1	1:K:34:ASP:N	2.35	0.57
1:L:79:VAL:HG23	1:L:130:LEU:HB3	1.87	0.57
1:N:79:VAL:HG23	1:N:130:LEU:HB3	1.87	0.57
1:A:200:GLN:HE21	1:A:231:GLN:CB	2.17	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:79:VAL:HG23	1:I:130:LEU:HB3	1.87	0.56
1:B:79:VAL:HG23	1:B:130:LEU:HB3	1.87	0.56
1:G:79:VAL:HG23	1:G:130:LEU:HB3	1.87	0.56
1:I:200:GLN:CD	1:I:299:LEU:HB2	2.25	0.56
1:E:286:ASN:ND2	1:E:289:GLU:OE2	2.37	0.56
1:M:286:ASN:ND2	1:M:289:GLU:OE2	2.37	0.56
1:F:286:ASN:ND2	1:F:289:GLU:OE2	2.37	0.56
1:M:79:VAL:HG23	1:M:130:LEU:HB3	1.87	0.56
1:A:79:VAL:HG23	1:A:130:LEU:HB3	1.87	0.56
1:E:79:VAL:HG23	1:E:130:LEU:HB3	1.87	0.56
1:B:31:ARG:O	1:B:35:LEU:CB	2.54	0.56
1:H:31:ARG:O	1:H:35:LEU:CB	2.54	0.56
1:A:31:ARG:O	1:A:35:LEU:CB	2.54	0.55
1:D:79:VAL:HG23	1:D:130:LEU:HB3	1.87	0.55
1:J:31:ARG:O	1:J:35:LEU:CB	2.54	0.55
1:J:79:VAL:HG23	1:J:130:LEU:HB3	1.87	0.55
1:N:31:ARG:O	1:N:35:LEU:CB	2.54	0.55
1:M:31:ARG:O	1:M:35:LEU:CB	2.54	0.55
2:O:18:DA:H1'	2:O:19:DC:H5'	1.88	0.55
1:H:286:ASN:ND2	1:H:289:GLU:OE2	2.37	0.55
1:C:31:ARG:O	1:C:35:LEU:CB	2.54	0.55
1:E:31:ARG:O	1:E:35:LEU:CB	2.54	0.55
1:F:31:ARG:O	1:F:35:LEU:CB	2.54	0.55
1:J:286:ASN:ND2	1:J:289:GLU:OE2	2.37	0.55
1:L:31:ARG:O	1:L:35:LEU:CB	2.54	0.54
1:G:31:ARG:O	1:G:35:LEU:CB	2.54	0.54
1:G:133:ILE:HB	1:G:168:ILE:HD13	1.90	0.54
1:I:31:ARG:O	1:I:35:LEU:CB	2.54	0.54
1:D:32:CYS:HG	1:D:43:THR:HG1	1.35	0.54
1:E:133:ILE:HB	1:E:168:ILE:HD13	1.90	0.54
1:K:31:ARG:O	1:K:35:LEU:CB	2.54	0.54
1:C:139:LEU:HD22	1:C:151:VAL:HG21	1.90	0.54
1:F:139:LEU:HD22	1:F:151:VAL:HG21	1.90	0.54
1:M:199:TYR:HD2	1:M:201:GLY:N	2.04	0.54
1:G:139:LEU:HD22	1:G:151:VAL:HG21	1.90	0.54
1:I:200:GLN:OE1	1:I:299:LEU:O	2.26	0.54
1:K:139:LEU:HD22	1:K:151:VAL:HG21	1.90	0.54
1:M:199:TYR:CZ	1:M:204:GLY:CA	2.91	0.54
1:M:133:ILE:HB	1:M:168:ILE:HD13	1.90	0.54
1:N:139:LEU:HD22	1:N:151:VAL:HG21	1.90	0.54
1:C:133:ILE:HB	1:C:168:ILE:HD13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:31:ARG:O	1:D:35:LEU:CB	2.54	0.54
1:D:139:LEU:HD22	1:D:151:VAL:HG21	1.90	0.54
1:M:199:TYR:CD2	1:M:201:GLY:N	2.76	0.54
1:A:133:ILE:HB	1:A:168:ILE:HD13	1.90	0.53
1:J:133:ILE:HB	1:J:168:ILE:HD13	1.90	0.53
1:M:139:LEU:HD22	1:M:151:VAL:HG21	1.90	0.53
1:N:199:TYR:CZ	1:N:204:GLY:HA3	2.44	0.53
1:B:139:LEU:HD22	1:B:151:VAL:HG21	1.90	0.53
1:E:139:LEU:HD22	1:E:151:VAL:HG21	1.90	0.53
1:M:199:TYR:OH	1:M:202:GLY:O	2.26	0.53
1:A:6:GLU:HB3	1:G:31:ARG:HH12	1.74	0.53
1:D:91:VAL:HB	1:D:112:LEU:HB2	1.91	0.53
1:I:139:LEU:HD22	1:I:151:VAL:HG21	1.90	0.53
1:J:91:VAL:HB	1:J:112:LEU:HB2	1.91	0.53
1:K:133:ILE:HB	1:K:168:ILE:HD13	1.90	0.53
1:L:91:VAL:HB	1:L:112:LEU:HB2	1.91	0.53
1:L:153:ASN:OD1	1:L:181:ASN:ND2	2.42	0.53
1:F:153:ASN:OD1	1:F:181:ASN:ND2	2.42	0.53
1:H:91:VAL:HB	1:H:112:LEU:HB2	1.91	0.53
1:I:133:ILE:HB	1:I:168:ILE:HD13	1.90	0.53
1:N:153:ASN:OD1	1:N:181:ASN:ND2	2.42	0.53
1:K:32:CYS:SG	1:K:43:THR:OG1	2.55	0.53
1:A:91:VAL:HB	1:A:112:LEU:HB2	1.91	0.53
1:G:91:VAL:HB	1:G:112:LEU:HB2	1.91	0.53
1:H:133:ILE:HB	1:H:168:ILE:HD13	1.90	0.53
1:M:199:TYR:HE2	1:M:202:GLY:H	0.79	0.53
1:N:143:ARG:NH2	3:P:22:DT:OP1	2.41	0.53
1:C:153:ASN:OD1	1:C:181:ASN:ND2	2.42	0.53
1:E:153:ASN:OD1	1:E:181:ASN:ND2	2.42	0.53
1:H:139:LEU:HD22	1:H:151:VAL:HG21	1.90	0.53
1:H:153:ASN:OD1	1:H:181:ASN:ND2	2.42	0.53
1:B:133:ILE:HB	1:B:168:ILE:HD13	1.90	0.52
1:F:133:ILE:HB	1:F:168:ILE:HD13	1.90	0.52
1:L:133:ILE:HB	1:L:168:ILE:HD13	1.90	0.52
1:M:91:VAL:HB	1:M:112:LEU:HB2	1.91	0.52
1:D:153:ASN:OD1	1:D:181:ASN:ND2	2.42	0.52
1:E:91:VAL:HB	1:E:112:LEU:HB2	1.91	0.52
1:J:153:ASN:OD1	1:J:181:ASN:ND2	2.42	0.52
1:A:108:TYR:CE1	1:G:112:LEU:HD21	2.44	0.52
1:A:153:ASN:OD1	1:A:181:ASN:ND2	2.42	0.52
1:B:91:VAL:HB	1:B:112:LEU:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:153:ASN:OD1	1:M:181:ASN:ND2	2.42	0.52
1:B:153:ASN:OD1	1:B:181:ASN:ND2	2.42	0.52
1:G:153:ASN:OD1	1:G:181:ASN:ND2	2.42	0.52
1:L:139:LEU:HD22	1:L:151:VAL:HG21	1.90	0.52
1:N:133:ILE:HB	1:N:168:ILE:HD13	1.90	0.52
1:D:133:ILE:HB	1:D:168:ILE:HD13	1.90	0.52
1:I:153:ASN:OD1	1:I:181:ASN:ND2	2.42	0.52
1:J:139:LEU:HD22	1:J:151:VAL:HG21	1.90	0.52
1:K:153:ASN:OD1	1:K:181:ASN:ND2	2.42	0.52
1:A:139:LEU:HD22	1:A:151:VAL:HG21	1.90	0.52
1:F:91:VAL:HB	1:F:112:LEU:HB2	1.91	0.52
1:N:200:GLN:OE1	1:N:231:GLN:CA	2.57	0.52
1:C:91:VAL:HB	1:C:112:LEU:HB2	1.91	0.52
1:K:91:VAL:HB	1:K:112:LEU:HB2	1.91	0.52
1:D:26:LEU:HA	1:D:29:MET:HG3	1.92	0.52
1:M:26:LEU:HA	1:M:29:MET:HG3	1.93	0.52
1:N:91:VAL:HB	1:N:112:LEU:HB2	1.91	0.52
1:B:26:LEU:HA	1:B:29:MET:HG3	1.93	0.51
1:H:149:THR:O	1:H:149:THR:OG1	2.27	0.51
1:I:91:VAL:HB	1:I:112:LEU:HB2	1.91	0.51
1:H:26:LEU:HA	1:H:29:MET:HG3	1.92	0.51
1:J:26:LEU:HA	1:J:29:MET:HG3	1.93	0.51
1:F:32:CYS:SG	1:F:43:THR:OG1	2.55	0.51
1:L:26:LEU:HA	1:L:29:MET:HG3	1.92	0.51
1:E:26:LEU:HA	1:E:29:MET:HG3	1.92	0.51
1:G:26:LEU:HA	1:G:29:MET:HG3	1.92	0.51
1:C:26:LEU:HA	1:C:29:MET:HG3	1.92	0.51
1:N:200:GLN:HE21	1:N:200:GLN:CA	2.23	0.51
1:F:26:LEU:HA	1:F:29:MET:HG3	1.93	0.51
1:D:32:CYS:SG	1:D:43:THR:OG1	2.55	0.51
1:M:199:TYR:CE1	1:M:204:GLY:CA	2.94	0.51
1:M:199:TYR:CE1	1:M:204:GLY:HA3	2.46	0.50
1:M:199:TYR:HD2	1:M:201:GLY:H	1.59	0.50
1:F:143:ARG:NH2	2:O:19:DC:OP1	2.37	0.50
1:G:271:PHE:HA	1:G:274:LYS:HG3	1.94	0.50
1:I:26:LEU:HA	1:I:29:MET:HG3	1.93	0.50
1:K:26:LEU:HA	1:K:29:MET:HG3	1.92	0.50
1:K:271:PHE:HA	1:K:274:LYS:HG3	1.94	0.50
1:C:271:PHE:HA	1:C:274:LYS:HG3	1.94	0.50
1:H:114:ARG:NH2	1:I:108:TYR:HA	2.25	0.50
1:J:271:PHE:HA	1:J:274:LYS:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:149:THR:O	1:M:149:THR:OG1	2.27	0.50
1:A:200:GLN:HE22	1:A:231:GLN:HB2	1.72	0.50
1:H:32:CYS:SG	1:H:43:THR:OG1	2.55	0.50
1:N:199:TYR:C	1:N:199:TYR:CD2	2.85	0.50
1:L:149:THR:O	1:L:149:THR:OG1	2.27	0.49
1:A:26:LEU:HA	1:A:29:MET:HG3	1.93	0.49
1:H:271:PHE:HA	1:H:274:LYS:HG3	1.94	0.49
1:N:26:LEU:HA	1:N:29:MET:HG3	1.93	0.49
1:A:271:PHE:HA	1:A:274:LYS:HG3	1.94	0.49
1:N:271:PHE:HA	1:N:274:LYS:HG3	1.94	0.49
1:B:271:PHE:HA	1:B:274:LYS:HG3	1.94	0.49
1:D:149:THR:O	1:D:149:THR:OG1	2.27	0.49
1:G:143:ARG:NH2	2:O:18:DA:OP1	2.43	0.49
1:D:271:PHE:HA	1:D:274:LYS:HG3	1.94	0.49
1:M:271:PHE:HA	1:M:274:LYS:HG3	1.94	0.49
1:C:214:ASP:HA	1:C:217:LEU:HD12	1.95	0.49
1:E:271:PHE:HA	1:E:274:LYS:HG3	1.94	0.49
1:F:271:PHE:HA	1:F:274:LYS:HG3	1.94	0.49
1:G:214:ASP:HA	1:G:217:LEU:HD12	1.95	0.49
1:M:190:ILE:HG12	1:N:275:LEU:HD23	1.95	0.49
1:K:214:ASP:HA	1:K:217:LEU:HD12	1.95	0.48
1:K:187:ARG:NH2	4:L:401:ATP:O2G	2.38	0.48
1:L:271:PHE:HA	1:L:274:LYS:HG3	1.94	0.48
1:A:108:TYR:CZ	1:G:112:LEU:HD21	2.49	0.48
1:I:271:PHE:HA	1:I:274:LYS:HG3	1.94	0.48
1:K:31:ARG:NH2	1:L:251:GLN:OE1	2.46	0.48
1:M:198:SER:O	1:M:235:TYR:OH	2.30	0.48
1:F:153:ASN:ND2	1:G:86:ASP:OD1	2.46	0.48
1:I:32:CYS:SG	1:I:43:THR:OG1	2.55	0.48
1:B:200:GLN:HE21	1:B:299:LEU:CD1	2.08	0.48
1:F:149:THR:O	1:F:149:THR:OG1	2.27	0.48
1:N:214:ASP:HA	1:N:217:LEU:HD12	1.95	0.48
1:B:214:ASP:HA	1:B:217:LEU:HD12	1.95	0.48
1:J:214:ASP:HA	1:J:217:LEU:HD12	1.95	0.48
1:M:214:ASP:HA	1:M:217:LEU:HD12	1.95	0.48
1:F:214:ASP:HA	1:F:217:LEU:HD12	1.95	0.47
1:L:214:ASP:HA	1:L:217:LEU:HD12	1.95	0.47
1:M:199:TYR:OH	1:M:202:GLY:C	2.52	0.47
1:A:214:ASP:HA	1:A:217:LEU:HD12	1.95	0.47
1:H:200:GLN:HG3	1:H:235:TYR:HB3	1.95	0.47
1:I:243:ARG:O	1:I:247:ASN:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:214:ASP:HA	1:D:217:LEU:HD12	1.95	0.47
1:D:135:GLU:OE1	1:D:137:GLN:NE2	2.41	0.47
1:D:198:SER:O	1:D:235:TYR:OH	2.30	0.47
1:E:214:ASP:HA	1:E:217:LEU:HD12	1.95	0.47
1:I:214:ASP:HA	1:I:217:LEU:HD12	1.95	0.47
1:M:185:HIS:NE2	1:N:279:ASP:O	2.47	0.47
1:B:211:GLU:HA	1:B:214:ASP:HB2	1.97	0.47
1:K:211:GLU:HA	1:K:214:ASP:HB2	1.97	0.47
1:C:243:ARG:O	1:C:247:ASN:HB2	2.14	0.47
1:E:243:ARG:O	1:E:247:ASN:HB2	2.14	0.47
1:F:198:SER:O	1:F:235:TYR:OH	2.30	0.47
1:F:211:GLU:HA	1:F:214:ASP:HB2	1.97	0.47
1:K:135:GLU:OE1	1:K:137:GLN:NE2	2.41	0.47
1:N:198:SER:O	1:N:235:TYR:OH	2.30	0.47
1:H:243:ARG:O	1:H:247:ASN:HB2	2.14	0.47
1:J:211:GLU:HA	1:J:214:ASP:HB2	1.97	0.47
1:K:149:THR:O	1:K:149:THR:OG1	2.27	0.47
1:K:198:SER:O	1:K:235:TYR:OH	2.30	0.47
1:L:35:LEU:HD11	1:M:254:ILE:HG12	1.96	0.47
1:M:243:ARG:O	1:M:247:ASN:HB2	2.14	0.47
1:N:199:TYR:HH	1:N:204:GLY:HA2	1.73	0.47
1:B:243:ARG:O	1:B:247:ASN:HB2	2.14	0.47
1:L:135:GLU:OE1	1:L:137:GLN:NE2	2.41	0.47
1:A:211:GLU:HA	1:A:214:ASP:HB2	1.97	0.47
1:C:211:GLU:HA	1:C:214:ASP:HB2	1.97	0.47
1:G:243:ARG:O	1:G:247:ASN:HB2	2.14	0.47
1:H:214:ASP:HA	1:H:217:LEU:HD12	1.95	0.47
1:I:211:GLU:HA	1:I:214:ASP:HB2	1.97	0.47
1:N:243:ARG:O	1:N:247:ASN:HB2	2.14	0.47
1:H:211:GLU:HA	1:H:214:ASP:HB2	1.97	0.46
1:K:243:ARG:O	1:K:247:ASN:HB2	2.14	0.46
1:L:243:ARG:O	1:L:247:ASN:HB2	2.14	0.46
1:F:243:ARG:O	1:F:247:ASN:HB2	2.14	0.46
1:J:198:SER:O	1:J:235:TYR:OH	2.30	0.46
1:N:200:GLN:O	1:N:200:GLN:HG3	2.14	0.46
1:G:211:GLU:HA	1:G:214:ASP:HB2	1.97	0.46
1:M:211:GLU:HA	1:M:214:ASP:HB2	1.97	0.46
1:N:211:GLU:HA	1:N:214:ASP:HB2	1.97	0.46
1:C:198:SER:O	1:C:235:TYR:OH	2.30	0.46
1:A:243:ARG:O	1:A:247:ASN:HB2	2.14	0.46
1:D:243:ARG:O	1:D:247:ASN:HB2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:135:GLU:OE1	1:N:137:GLN:NE2	2.41	0.46
1:C:187:ARG:NH1	4:D:401:ATP:O3G	2.44	0.46
1:B:135:GLU:OE1	1:B:137:GLN:NE2	2.41	0.46
1:G:149:THR:O	1:G:149:THR:OG1	2.27	0.46
1:J:243:ARG:O	1:J:247:ASN:HB2	2.14	0.46
1:E:198:SER:O	1:E:235:TYR:OH	2.30	0.45
1:B:149:THR:O	1:B:149:THR:OG1	2.27	0.45
1:E:211:GLU:HA	1:E:214:ASP:HB2	1.97	0.45
1:G:37:ASP:OD1	1:G:37:ASP:N	2.45	0.45
1:J:149:THR:O	1:J:149:THR:OG1	2.27	0.45
1:L:211:GLU:HA	1:L:214:ASP:HB2	1.97	0.45
1:D:211:GLU:HA	1:D:214:ASP:HB2	1.97	0.45
1:H:200:GLN:OE1	1:H:235:TYR:HB2	2.14	0.45
1:B:198:SER:O	1:B:235:TYR:OH	2.30	0.45
1:I:200:GLN:OE1	1:I:200:GLN:N	2.50	0.45
1:I:198:SER:O	1:I:235:TYR:OH	2.30	0.45
1:H:135:GLU:OE1	1:H:137:GLN:NE2	2.41	0.45
1:J:32:CYS:SG	1:J:43:THR:OG1	2.55	0.45
1:M:135:GLU:OE1	1:M:137:GLN:NE2	2.41	0.45
2:O:18:DA:N6	3:P:38:DG:O6	2.50	0.45
1:A:32:CYS:SG	1:A:43:THR:OG1	2.55	0.44
1:A:149:THR:O	1:A:149:THR:OG1	2.27	0.44
1:G:32:CYS:SG	1:G:43:THR:OG1	2.55	0.44
1:K:150:GLN:NE2	1:L:142:GLU:OE1	2.51	0.44
1:D:35:LEU:HD11	1:E:254:ILE:HG12	1.99	0.44
1:D:200:GLN:OE1	1:D:231:GLN:C	2.56	0.44
3:P:35:DG:H2''	3:P:36:DC:O4'	2.18	0.44
1:J:302:PRO:HA	1:J:303:PRO:HD3	1.88	0.44
1:G:302:PRO:HA	1:G:303:PRO:HD3	1.88	0.44
1:E:149:THR:O	1:E:149:THR:OG1	2.27	0.44
1:C:149:THR:O	1:C:149:THR:OG1	2.27	0.43
1:A:198:SER:O	1:A:235:TYR:OH	2.30	0.43
1:L:233:LYS:H	1:L:233:LYS:HG2	1.64	0.43
1:B:249:ILE:HD13	1:B:249:ILE:HA	1.87	0.43
1:G:249:ILE:HD13	1:G:249:ILE:HA	1.87	0.43
1:I:59:ILE:O	1:I:63:LEU:HG	2.19	0.43
1:L:35:LEU:CD1	1:M:254:ILE:HG12	2.48	0.43
1:B:37:ASP:OD1	1:B:37:ASP:N	2.45	0.43
1:F:233:LYS:H	1:F:233:LYS:HG2	1.64	0.43
1:H:198:SER:O	1:H:235:TYR:OH	2.30	0.43
1:I:149:THR:O	1:I:149:THR:OG1	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:249:ILE:HD13	1:J:249:ILE:HA	1.87	0.43
1:L:59:ILE:O	1:L:63:LEU:HG	2.19	0.43
1:L:285:LYS:HD2	1:L:285:LYS:HA	1.87	0.43
1:N:32:CYS:SG	1:N:43:THR:OG1	2.55	0.43
1:I:285:LYS:HD2	1:I:285:LYS:HA	1.87	0.43
1:B:59:ILE:O	1:B:63:LEU:HG	2.19	0.43
1:B:210:LEU:HB3	1:B:226:ALA:HB2	2.01	0.43
1:G:59:ILE:O	1:G:63:LEU:HG	2.19	0.43
1:J:59:ILE:O	1:J:63:LEU:HG	2.19	0.43
1:K:59:ILE:O	1:K:63:LEU:HG	2.19	0.43
1:A:59:ILE:O	1:A:63:LEU:HG	2.19	0.43
1:C:210:LEU:HB3	1:C:226:ALA:HB2	2.01	0.43
1:E:210:LEU:HB3	1:E:226:ALA:HB2	2.01	0.43
1:F:210:LEU:HB3	1:F:226:ALA:HB2	2.01	0.43
1:G:210:LEU:HB3	1:G:226:ALA:HB2	2.01	0.43
1:H:77:ILE:HD12	1:H:77:ILE:HA	1.94	0.43
1:H:114:ARG:NH1	1:I:108:TYR:HD1	2.16	0.43
1:J:210:LEU:HB3	1:J:226:ALA:HB2	2.01	0.43
1:K:210:LEU:HB3	1:K:226:ALA:HB2	2.01	0.43
1:D:59:ILE:O	1:D:63:LEU:HG	2.19	0.42
1:H:59:ILE:O	1:H:63:LEU:HG	2.19	0.42
1:M:210:LEU:HB3	1:M:226:ALA:HB2	2.01	0.42
1:D:285:LYS:HD2	1:D:285:LYS:HA	1.87	0.42
1:D:210:LEU:HB3	1:D:226:ALA:HB2	2.01	0.42
1:N:59:ILE:O	1:N:63:LEU:HG	2.19	0.42
1:N:210:LEU:HB3	1:N:226:ALA:HB2	2.01	0.42
1:H:210:LEU:HB3	1:H:226:ALA:HB2	2.01	0.42
1:C:59:ILE:O	1:C:63:LEU:HG	2.19	0.42
1:F:59:ILE:O	1:F:63:LEU:HG	2.19	0.42
1:B:32:CYS:SG	1:B:43:THR:OG1	2.55	0.42
1:E:59:ILE:O	1:E:63:LEU:HG	2.19	0.42
1:G:200:GLN:NE2	1:G:200:GLN:C	2.73	0.42
1:F:80:LEU:HD21	1:F:101:MET:HB3	2.02	0.42
1:I:210:LEU:HB3	1:I:226:ALA:HB2	2.01	0.42
1:J:80:LEU:HD21	1:J:101:MET:HB3	2.02	0.42
1:L:32:CYS:SG	1:L:43:THR:OG1	2.55	0.42
1:N:199:TYR:CD2	1:N:199:TYR:O	2.73	0.42
1:A:80:LEU:HD21	1:A:101:MET:HB3	2.02	0.42
1:C:302:PRO:HA	1:C:303:PRO:HD3	1.88	0.42
1:G:135:GLU:OE1	1:G:137:GLN:NE2	2.41	0.42
1:H:135:GLU:HB3	1:H:138:HIS:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:210:LEU:HB3	1:L:226:ALA:HB2	2.01	0.42
1:D:135:GLU:HB3	1:D:138:HIS:CD2	2.55	0.42
1:I:302:PRO:HA	1:I:303:PRO:HD3	1.88	0.42
1:M:59:ILE:O	1:M:63:LEU:HG	2.19	0.42
1:F:135:GLU:HB3	1:F:138:HIS:CD2	2.55	0.42
1:H:80:LEU:HD21	1:H:101:MET:HB3	2.02	0.42
1:J:135:GLU:HB3	1:J:138:HIS:CD2	2.55	0.42
1:K:80:LEU:HD21	1:K:101:MET:HB3	2.02	0.42
1:D:77:ILE:HD12	1:D:77:ILE:HA	1.95	0.41
1:F:77:ILE:HD12	1:F:77:ILE:HA	1.95	0.41
1:G:48:TYR:HE2	1:G:191:GLN:HB3	1.85	0.41
1:I:80:LEU:HD21	1:I:101:MET:HB3	2.02	0.41
1:K:48:TYR:HE2	1:K:191:GLN:HB3	1.85	0.41
1:L:135:GLU:HB3	1:L:138:HIS:CD2	2.55	0.41
1:N:80:LEU:HD21	1:N:101:MET:HB3	2.02	0.41
1:A:48:TYR:HE2	1:A:191:GLN:HB3	1.85	0.41
1:B:135:GLU:HB3	1:B:138:HIS:CD2	2.55	0.41
1:C:48:TYR:HE2	1:C:191:GLN:HB3	1.85	0.41
1:F:302:PRO:HA	1:F:303:PRO:HD3	1.88	0.41
1:G:198:SER:O	1:G:235:TYR:OH	2.30	0.41
1:M:48:TYR:HE2	1:M:191:GLN:HB3	1.85	0.41
1:E:48:TYR:HE2	1:E:191:GLN:HB3	1.85	0.41
1:E:135:GLU:HB3	1:E:138:HIS:CD2	2.55	0.41
1:F:231:GLN:HA	1:F:234:LEU:HB2	2.03	0.41
1:G:135:GLU:HB3	1:G:138:HIS:CD2	2.55	0.41
1:H:48:TYR:HE2	1:H:191:GLN:HB3	1.85	0.41
1:L:48:TYR:HE2	1:L:191:GLN:HB3	1.85	0.41
1:B:231:GLN:HA	1:B:234:LEU:HB2	2.03	0.41
1:G:231:GLN:HA	1:G:234:LEU:HB2	2.03	0.41
1:H:233:LYS:H	1:H:233:LYS:HG2	1.64	0.41
1:L:37:ASP:OD1	1:L:37:ASP:N	2.45	0.41
1:L:77:ILE:HD12	1:L:77:ILE:HA	1.95	0.41
1:B:48:TYR:HE2	1:B:191:GLN:HB3	1.85	0.41
1:D:233:LYS:H	1:D:233:LYS:HG2	1.64	0.41
1:H:302:PRO:HA	1:H:303:PRO:HD3	1.88	0.41
1:A:210:LEU:HB3	1:A:226:ALA:HB2	2.01	0.41
1:E:231:GLN:HA	1:E:234:LEU:HB2	2.03	0.41
1:G:80:LEU:HD21	1:G:101:MET:HB3	2.02	0.41
1:M:37:ASP:OD1	1:M:37:ASP:N	2.45	0.41
1:M:285:LYS:HD2	1:M:285:LYS:HA	1.87	0.41
1:C:80:LEU:HD21	1:C:101:MET:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:77:ILE:HD12	1:G:77:ILE:HA	1.95	0.41
1:N:135:GLU:HB3	1:N:138:HIS:CD2	2.55	0.41
1:B:80:LEU:HD21	1:B:101:MET:HB3	2.02	0.41
1:C:135:GLU:HB3	1:C:138:HIS:CD2	2.55	0.41
1:C:309:GLU:OE1	1:C:309:GLU:N	2.51	0.41
1:D:48:TYR:HE2	1:D:191:GLN:HB3	1.85	0.41
1:E:37:ASP:OD1	1:E:37:ASP:N	2.45	0.41
1:J:135:GLU:OE1	1:J:137:GLN:NE2	2.41	0.41
1:M:135:GLU:HB3	1:M:138:HIS:CD2	2.55	0.41
1:A:135:GLU:HB3	1:A:138:HIS:CD2	2.55	0.41
1:A:135:GLU:OE1	1:A:137:GLN:NE2	2.41	0.41
1:D:231:GLN:HA	1:D:234:LEU:HB2	2.03	0.41
1:G:82:ILE:HD13	1:G:82:ILE:HA	1.90	0.41
1:I:190:ILE:HG12	1:J:275:LEU:HD23	2.02	0.41
1:K:200:GLN:OE1	1:K:231:GLN:O	2.39	0.41
1:L:231:GLN:HA	1:L:234:LEU:HB2	2.03	0.41
1:N:149:THR:O	1:N:149:THR:OG1	2.27	0.41
1:N:200:GLN:O	1:N:200:GLN:CG	2.69	0.41
1:A:231:GLN:HA	1:A:234:LEU:HB2	2.03	0.41
1:E:135:GLU:OE1	1:E:137:GLN:NE2	2.41	0.41
1:F:146:ARG:NH1	1:G:143:ARG:HG2	2.36	0.41
1:K:135:GLU:HB3	1:K:138:HIS:CD2	2.55	0.41
1:L:80:LEU:HD21	1:L:101:MET:HB3	2.02	0.41
1:M:77:ILE:HD12	1:M:77:ILE:HA	1.95	0.41
1:M:199:TYR:CE2	1:M:202:GLY:N	2.50	0.41
1:N:48:TYR:HE2	1:N:191:GLN:HB3	1.85	0.41
1:A:205:VAL:H	1:A:205:VAL:HG12	1.66	0.40
1:C:231:GLN:HA	1:C:234:LEU:HB2	2.03	0.40
1:I:135:GLU:HB3	1:I:138:HIS:CD2	2.55	0.40
1:I:231:GLN:HA	1:I:234:LEU:HB2	2.03	0.40
1:J:48:TYR:HE2	1:J:191:GLN:HB3	1.85	0.40
1:J:231:GLN:HA	1:J:234:LEU:HB2	2.03	0.40
1:M:231:GLN:HA	1:M:234:LEU:HB2	2.03	0.40
1:I:48:TYR:HE2	1:I:191:GLN:HB3	1.85	0.40
1:J:37:ASP:OD1	1:J:37:ASP:N	2.45	0.40
1:M:82:ILE:HD13	1:M:82:ILE:HA	1.90	0.40
1:B:302:PRO:HA	1:B:303:PRO:HD3	1.88	0.40
1:C:135:GLU:OE1	1:C:137:GLN:NE2	2.41	0.40
1:F:143:ARG:NH1	2:O:19:DC:H5''	2.36	0.40
1:J:187:ARG:NH1	4:K:401:ATP:O3G	2.49	0.40
1:M:199:TYR:CZ	1:M:204:GLY:HA3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:GLU:OE1	1:B:309:GLU:N	2.51	0.40
1:C:95:ARG:O	1:C:99:VAL:HG12	2.22	0.40
1:D:302:PRO:HA	1:D:303:PRO:HD3	1.88	0.40
1:E:80:LEU:HD21	1:E:101:MET:HB3	2.02	0.40
1:C:82:ILE:HD13	1:C:82:ILE:HA	1.90	0.40
1:D:80:LEU:HD21	1:D:101:MET:HB3	2.02	0.40
1:H:95:ARG:O	1:H:99:VAL:HG12	2.22	0.40
1:I:95:ARG:O	1:I:99:VAL:HG12	2.22	0.40
1:K:95:ARG:O	1:K:99:VAL:HG12	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	309/311 (99%)	275 (89%)	34 (11%)	0	100	100
1	B	309/311 (99%)	275 (89%)	34 (11%)	0	100	100
1	C	309/311 (99%)	275 (89%)	34 (11%)	0	100	100
1	D	309/311 (99%)	275 (89%)	34 (11%)	0	100	100
1	E	309/311 (99%)	275 (89%)	34 (11%)	0	100	100
1	F	309/311 (99%)	275 (89%)	34 (11%)	0	100	100
1	G	309/311 (99%)	275 (89%)	34 (11%)	0	100	100
1	H	309/311 (99%)	275 (89%)	34 (11%)	0	100	100
1	I	309/311 (99%)	275 (89%)	34 (11%)	0	100	100
1	J	309/311 (99%)	275 (89%)	34 (11%)	0	100	100
1	K	309/311 (99%)	275 (89%)	34 (11%)	0	100	100
1	L	309/311 (99%)	275 (89%)	34 (11%)	0	100	100
1	M	309/311 (99%)	274 (89%)	35 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	309/311 (99%)	274 (89%)	35 (11%)	0	100	100
All	All	4326/4354 (99%)	3848 (89%)	478 (11%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	268/268 (100%)	207 (77%)	61 (23%)	1	6
1	B	268/268 (100%)	206 (77%)	62 (23%)	1	6
1	C	268/268 (100%)	207 (77%)	61 (23%)	1	6
1	D	268/268 (100%)	207 (77%)	61 (23%)	1	6
1	E	268/268 (100%)	206 (77%)	62 (23%)	1	6
1	F	268/268 (100%)	206 (77%)	62 (23%)	1	6
1	G	268/268 (100%)	206 (77%)	62 (23%)	1	6
1	H	268/268 (100%)	207 (77%)	61 (23%)	1	6
1	I	268/268 (100%)	207 (77%)	61 (23%)	1	6
1	J	268/268 (100%)	207 (77%)	61 (23%)	1	6
1	K	268/268 (100%)	207 (77%)	61 (23%)	1	6
1	L	268/268 (100%)	206 (77%)	62 (23%)	1	6
1	M	268/268 (100%)	206 (77%)	62 (23%)	1	6
1	N	268/268 (100%)	206 (77%)	62 (23%)	1	6
All	All	3752/3752 (100%)	2891 (77%)	861 (23%)	3	6

All (861) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ARG
1	A	29	MET

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Mol	Chain	Res	Type
1	A	32	CYS
1	A	34	ASP
1	A	39	GLU
1	A	40	SER
1	A	41	GLU
1	A	51	SER
1	A	59	ILE
1	A	63	LEU
1	A	64	ASN
1	A	83	GLU
1	A	100	GLU
1	A	105	LEU
1	A	116	THR
1	A	117	LYS
1	A	119	LEU
1	A	121	GLU
1	A	123	ILE
1	A	134	ASP
1	A	143	ARG
1	A	147	VAL
1	A	149	THR
1	A	155	LEU
1	A	156	LYS
1	A	163	LYS
1	A	178	LEU
1	A	189	SER
1	A	193	GLU
1	A	194	LEU
1	A	203	ARG
1	A	208	THR
1	A	210	LEU
1	A	211	GLU
1	A	220	GLU
1	A	221	LYS
1	A	228	GLU
1	A	233	LYS
1	A	234	LEU
1	A	248	LEU
1	A	249	ILE
1	A	257	ILE
1	A	258	ASP
1	A	260	GLN

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Mol	Chain	Res	Type
1	A	262	GLU
1	A	263	THR
1	A	265	THR
1	A	266	GLU
1	A	267	GLU
1	A	275	LEU
1	A	277	SER
1	A	279	ASP
1	A	286	ASN
1	A	289	GLU
1	A	293	GLU
1	A	296	GLU
1	A	297	ASP
1	A	298	MET
1	A	305	ASP
1	A	309	GLU
1	A	312	LEU
1	B	11	ARG
1	B	29	MET
1	B	32	CYS
1	B	34	ASP
1	B	39	GLU
1	B	40	SER
1	B	41	GLU
1	B	51	SER
1	B	59	ILE
1	B	63	LEU
1	B	64	ASN
1	B	83	GLU
1	B	100	GLU
1	B	105	LEU
1	B	116	THR
1	B	117	LYS
1	B	119	LEU
1	B	121	GLU
1	B	123	ILE
1	B	134	ASP
1	B	143	ARG
1	B	147	VAL
1	B	149	THR
1	B	155	LEU
1	B	156	LYS

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Mol	Chain	Res	Type
1	B	163	LYS
1	B	178	LEU
1	B	189	SER
1	B	193	GLU
1	B	194	LEU
1	B	200	GLN
1	B	203	ARG
1	B	208	THR
1	B	210	LEU
1	B	211	GLU
1	B	220	GLU
1	B	221	LYS
1	B	228	GLU
1	B	233	LYS
1	B	234	LEU
1	B	248	LEU
1	B	249	ILE
1	B	257	ILE
1	B	258	ASP
1	B	260	GLN
1	B	262	GLU
1	B	263	THR
1	B	265	THR
1	B	266	GLU
1	B	267	GLU
1	B	275	LEU
1	B	277	SER
1	B	279	ASP
1	B	286	ASN
1	B	289	GLU
1	B	293	GLU
1	B	296	GLU
1	B	297	ASP
1	B	298	MET
1	B	305	ASP
1	B	309	GLU
1	B	312	LEU
1	C	11	ARG
1	C	29	MET
1	C	32	CYS
1	C	34	ASP
1	C	39	GLU

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Mol	Chain	Res	Type
1	C	40	SER
1	C	41	GLU
1	C	51	SER
1	C	59	ILE
1	C	63	LEU
1	C	64	ASN
1	C	83	GLU
1	C	100	GLU
1	C	105	LEU
1	C	116	THR
1	C	117	LYS
1	C	119	LEU
1	C	121	GLU
1	C	123	ILE
1	C	134	ASP
1	C	143	ARG
1	C	147	VAL
1	C	149	THR
1	C	155	LEU
1	C	156	LYS
1	C	163	LYS
1	C	178	LEU
1	C	189	SER
1	C	193	GLU
1	C	194	LEU
1	C	203	ARG
1	C	208	THR
1	C	210	LEU
1	C	211	GLU
1	C	220	GLU
1	C	221	LYS
1	C	228	GLU
1	C	233	LYS
1	C	234	LEU
1	C	248	LEU
1	C	249	ILE
1	C	257	ILE
1	C	258	ASP
1	C	260	GLN
1	C	262	GLU
1	C	263	THR
1	C	265	THR

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Mol	Chain	Res	Type
1	C	266	GLU
1	C	267	GLU
1	C	275	LEU
1	C	277	SER
1	C	279	ASP
1	C	286	ASN
1	C	289	GLU
1	C	293	GLU
1	C	296	GLU
1	C	297	ASP
1	C	298	MET
1	C	305	ASP
1	C	309	GLU
1	C	312	LEU
1	D	11	ARG
1	D	29	MET
1	D	32	CYS
1	D	34	ASP
1	D	39	GLU
1	D	40	SER
1	D	41	GLU
1	D	51	SER
1	D	59	ILE
1	D	63	LEU
1	D	64	ASN
1	D	83	GLU
1	D	100	GLU
1	D	105	LEU
1	D	116	THR
1	D	117	LYS
1	D	119	LEU
1	D	121	GLU
1	D	123	ILE
1	D	134	ASP
1	D	143	ARG
1	D	147	VAL
1	D	149	THR
1	D	155	LEU
1	D	156	LYS
1	D	163	LYS
1	D	178	LEU
1	D	189	SER

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Mol	Chain	Res	Type
1	D	193	GLU
1	D	194	LEU
1	D	203	ARG
1	D	208	THR
1	D	210	LEU
1	D	211	GLU
1	D	220	GLU
1	D	221	LYS
1	D	228	GLU
1	D	233	LYS
1	D	234	LEU
1	D	248	LEU
1	D	249	ILE
1	D	257	ILE
1	D	258	ASP
1	D	260	GLN
1	D	262	GLU
1	D	263	THR
1	D	265	THR
1	D	266	GLU
1	D	267	GLU
1	D	275	LEU
1	D	277	SER
1	D	279	ASP
1	D	286	ASN
1	D	289	GLU
1	D	293	GLU
1	D	296	GLU
1	D	297	ASP
1	D	298	MET
1	D	305	ASP
1	D	309	GLU
1	D	312	LEU
1	E	11	ARG
1	E	29	MET
1	E	32	CYS
1	E	34	ASP
1	E	39	GLU
1	E	40	SER
1	E	41	GLU
1	E	51	SER
1	E	59	ILE

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Mol	Chain	Res	Type
1	E	63	LEU
1	E	64	ASN
1	E	83	GLU
1	E	100	GLU
1	E	105	LEU
1	E	116	THR
1	E	117	LYS
1	E	119	LEU
1	E	121	GLU
1	E	123	ILE
1	E	134	ASP
1	E	143	ARG
1	E	147	VAL
1	E	149	THR
1	E	155	LEU
1	E	156	LYS
1	E	163	LYS
1	E	178	LEU
1	E	189	SER
1	E	193	GLU
1	E	194	LEU
1	E	200	GLN
1	E	203	ARG
1	E	208	THR
1	E	210	LEU
1	E	211	GLU
1	E	220	GLU
1	E	221	LYS
1	E	228	GLU
1	E	233	LYS
1	E	234	LEU
1	E	248	LEU
1	E	249	ILE
1	E	257	ILE
1	E	258	ASP
1	E	260	GLN
1	E	262	GLU
1	E	263	THR
1	E	265	THR
1	E	266	GLU
1	E	267	GLU
1	E	275	LEU

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Mol	Chain	Res	Type
1	E	277	SER
1	E	279	ASP
1	E	286	ASN
1	E	289	GLU
1	E	293	GLU
1	E	296	GLU
1	E	297	ASP
1	E	298	MET
1	E	305	ASP
1	E	309	GLU
1	E	312	LEU
1	F	11	ARG
1	F	29	MET
1	F	32	CYS
1	F	34	ASP
1	F	39	GLU
1	F	40	SER
1	F	41	GLU
1	F	51	SER
1	F	59	ILE
1	F	63	LEU
1	F	64	ASN
1	F	83	GLU
1	F	100	GLU
1	F	105	LEU
1	F	116	THR
1	F	117	LYS
1	F	119	LEU
1	F	121	GLU
1	F	123	ILE
1	F	134	ASP
1	F	143	ARG
1	F	147	VAL
1	F	149	THR
1	F	155	LEU
1	F	156	LYS
1	F	163	LYS
1	F	178	LEU
1	F	189	SER
1	F	193	GLU
1	F	194	LEU
1	F	200	GLN

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Mol	Chain	Res	Type
1	F	203	ARG
1	F	208	THR
1	F	210	LEU
1	F	211	GLU
1	F	220	GLU
1	F	221	LYS
1	F	228	GLU
1	F	233	LYS
1	F	234	LEU
1	F	248	LEU
1	F	249	ILE
1	F	257	ILE
1	F	258	ASP
1	F	260	GLN
1	F	262	GLU
1	F	263	THR
1	F	265	THR
1	F	266	GLU
1	F	267	GLU
1	F	275	LEU
1	F	277	SER
1	F	279	ASP
1	F	286	ASN
1	F	289	GLU
1	F	293	GLU
1	F	296	GLU
1	F	297	ASP
1	F	298	MET
1	F	305	ASP
1	F	309	GLU
1	F	312	LEU
1	G	11	ARG
1	G	29	MET
1	G	32	CYS
1	G	34	ASP
1	G	39	GLU
1	G	40	SER
1	G	41	GLU
1	G	51	SER
1	G	59	ILE
1	G	63	LEU
1	G	64	ASN

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Mol	Chain	Res	Type
1	G	83	GLU
1	G	100	GLU
1	G	105	LEU
1	G	116	THR
1	G	117	LYS
1	G	119	LEU
1	G	121	GLU
1	G	123	ILE
1	G	134	ASP
1	G	143	ARG
1	G	147	VAL
1	G	149	THR
1	G	155	LEU
1	G	156	LYS
1	G	163	LYS
1	G	178	LEU
1	G	189	SER
1	G	193	GLU
1	G	194	LEU
1	G	200	GLN
1	G	203	ARG
1	G	208	THR
1	G	210	LEU
1	G	211	GLU
1	G	220	GLU
1	G	221	LYS
1	G	228	GLU
1	G	233	LYS
1	G	234	LEU
1	G	248	LEU
1	G	249	ILE
1	G	257	ILE
1	G	258	ASP
1	G	260	GLN
1	G	262	GLU
1	G	263	THR
1	G	265	THR
1	G	266	GLU
1	G	267	GLU
1	G	275	LEU
1	G	277	SER
1	G	279	ASP

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Mol	Chain	Res	Type
1	G	286	ASN
1	G	289	GLU
1	G	293	GLU
1	G	296	GLU
1	G	297	ASP
1	G	298	MET
1	G	305	ASP
1	G	309	GLU
1	G	312	LEU
1	H	11	ARG
1	H	29	MET
1	H	32	CYS
1	H	34	ASP
1	H	39	GLU
1	H	40	SER
1	H	41	GLU
1	H	51	SER
1	H	59	ILE
1	H	63	LEU
1	H	64	ASN
1	H	83	GLU
1	H	100	GLU
1	H	105	LEU
1	H	116	THR
1	H	117	LYS
1	H	119	LEU
1	H	121	GLU
1	H	123	ILE
1	H	134	ASP
1	H	143	ARG
1	H	147	VAL
1	H	149	THR
1	H	155	LEU
1	H	156	LYS
1	H	163	LYS
1	H	178	LEU
1	H	189	SER
1	H	193	GLU
1	H	194	LEU
1	H	203	ARG
1	H	208	THR
1	H	210	LEU

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Mol	Chain	Res	Type
1	H	211	GLU
1	H	220	GLU
1	H	221	LYS
1	H	228	GLU
1	H	233	LYS
1	H	234	LEU
1	H	248	LEU
1	H	249	ILE
1	H	257	ILE
1	H	258	ASP
1	H	260	GLN
1	H	262	GLU
1	H	263	THR
1	H	265	THR
1	H	266	GLU
1	H	267	GLU
1	H	275	LEU
1	H	277	SER
1	H	279	ASP
1	H	286	ASN
1	H	289	GLU
1	H	293	GLU
1	H	296	GLU
1	H	297	ASP
1	H	298	MET
1	H	305	ASP
1	H	309	GLU
1	H	312	LEU
1	I	11	ARG
1	I	29	MET
1	I	32	CYS
1	I	34	ASP
1	I	39	GLU
1	I	40	SER
1	I	41	GLU
1	I	51	SER
1	I	59	ILE
1	I	63	LEU
1	I	64	ASN
1	I	83	GLU
1	I	100	GLU
1	I	105	LEU

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Mol	Chain	Res	Type
1	I	116	THR
1	I	117	LYS
1	I	119	LEU
1	I	121	GLU
1	I	123	ILE
1	I	134	ASP
1	I	143	ARG
1	I	147	VAL
1	I	149	THR
1	I	155	LEU
1	I	156	LYS
1	I	163	LYS
1	I	178	LEU
1	I	189	SER
1	I	193	GLU
1	I	194	LEU
1	I	203	ARG
1	I	208	THR
1	I	210	LEU
1	I	211	GLU
1	I	220	GLU
1	I	221	LYS
1	I	228	GLU
1	I	233	LYS
1	I	234	LEU
1	I	248	LEU
1	I	249	ILE
1	I	257	ILE
1	I	258	ASP
1	I	260	GLN
1	I	262	GLU
1	I	263	THR
1	I	265	THR
1	I	266	GLU
1	I	267	GLU
1	I	275	LEU
1	I	277	SER
1	I	279	ASP
1	I	286	ASN
1	I	289	GLU
1	I	293	GLU
1	I	296	GLU

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Mol	Chain	Res	Type
1	I	297	ASP
1	I	298	MET
1	I	305	ASP
1	I	309	GLU
1	I	312	LEU
1	J	11	ARG
1	J	29	MET
1	J	32	CYS
1	J	34	ASP
1	J	39	GLU
1	J	40	SER
1	J	41	GLU
1	J	51	SER
1	J	59	ILE
1	J	63	LEU
1	J	64	ASN
1	J	83	GLU
1	J	100	GLU
1	J	105	LEU
1	J	116	THR
1	J	117	LYS
1	J	119	LEU
1	J	121	GLU
1	J	123	ILE
1	J	134	ASP
1	J	143	ARG
1	J	147	VAL
1	J	149	THR
1	J	155	LEU
1	J	156	LYS
1	J	163	LYS
1	J	178	LEU
1	J	189	SER
1	J	193	GLU
1	J	194	LEU
1	J	203	ARG
1	J	208	THR
1	J	210	LEU
1	J	211	GLU
1	J	220	GLU
1	J	221	LYS
1	J	228	GLU

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Mol	Chain	Res	Type
1	J	233	LYS
1	J	234	LEU
1	J	248	LEU
1	J	249	ILE
1	J	257	ILE
1	J	258	ASP
1	J	260	GLN
1	J	262	GLU
1	J	263	THR
1	J	265	THR
1	J	266	GLU
1	J	267	GLU
1	J	275	LEU
1	J	277	SER
1	J	279	ASP
1	J	286	ASN
1	J	289	GLU
1	J	293	GLU
1	J	296	GLU
1	J	297	ASP
1	J	298	MET
1	J	305	ASP
1	J	309	GLU
1	J	312	LEU
1	K	11	ARG
1	K	29	MET
1	K	32	CYS
1	K	34	ASP
1	K	39	GLU
1	K	40	SER
1	K	41	GLU
1	K	51	SER
1	K	59	ILE
1	K	63	LEU
1	K	64	ASN
1	K	83	GLU
1	K	100	GLU
1	K	105	LEU
1	K	116	THR
1	K	117	LYS
1	K	119	LEU
1	K	121	GLU

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Mol	Chain	Res	Type
1	K	123	ILE
1	K	134	ASP
1	K	143	ARG
1	K	147	VAL
1	K	149	THR
1	K	155	LEU
1	K	156	LYS
1	K	163	LYS
1	K	178	LEU
1	K	189	SER
1	K	193	GLU
1	K	194	LEU
1	K	203	ARG
1	K	208	THR
1	K	210	LEU
1	K	211	GLU
1	K	220	GLU
1	K	221	LYS
1	K	228	GLU
1	K	233	LYS
1	K	234	LEU
1	K	248	LEU
1	K	249	ILE
1	K	257	ILE
1	K	258	ASP
1	K	260	GLN
1	K	262	GLU
1	K	263	THR
1	K	265	THR
1	K	266	GLU
1	K	267	GLU
1	K	275	LEU
1	K	277	SER
1	K	279	ASP
1	K	286	ASN
1	K	289	GLU
1	K	293	GLU
1	K	296	GLU
1	K	297	ASP
1	K	298	MET
1	K	305	ASP
1	K	309	GLU

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Mol	Chain	Res	Type
1	K	312	LEU
1	L	11	ARG
1	L	29	MET
1	L	32	CYS
1	L	34	ASP
1	L	39	GLU
1	L	40	SER
1	L	41	GLU
1	L	51	SER
1	L	59	ILE
1	L	63	LEU
1	L	64	ASN
1	L	83	GLU
1	L	100	GLU
1	L	105	LEU
1	L	116	THR
1	L	117	LYS
1	L	119	LEU
1	L	121	GLU
1	L	123	ILE
1	L	134	ASP
1	L	143	ARG
1	L	147	VAL
1	L	149	THR
1	L	155	LEU
1	L	156	LYS
1	L	163	LYS
1	L	178	LEU
1	L	189	SER
1	L	193	GLU
1	L	194	LEU
1	L	200	GLN
1	L	203	ARG
1	L	208	THR
1	L	210	LEU
1	L	211	GLU
1	L	220	GLU
1	L	221	LYS
1	L	228	GLU
1	L	233	LYS
1	L	234	LEU
1	L	248	LEU

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Mol	Chain	Res	Type
1	L	249	ILE
1	L	257	ILE
1	L	258	ASP
1	L	260	GLN
1	L	262	GLU
1	L	263	THR
1	L	265	THR
1	L	266	GLU
1	L	267	GLU
1	L	275	LEU
1	L	277	SER
1	L	279	ASP
1	L	286	ASN
1	L	289	GLU
1	L	293	GLU
1	L	296	GLU
1	L	297	ASP
1	L	298	MET
1	L	305	ASP
1	L	309	GLU
1	L	312	LEU
1	M	11	ARG
1	M	29	MET
1	M	32	CYS
1	M	34	ASP
1	M	39	GLU
1	M	40	SER
1	M	41	GLU
1	M	51	SER
1	M	59	ILE
1	M	63	LEU
1	M	64	ASN
1	M	83	GLU
1	M	100	GLU
1	M	105	LEU
1	M	116	THR
1	M	117	LYS
1	M	119	LEU
1	M	121	GLU
1	M	123	ILE
1	M	134	ASP
1	M	143	ARG

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Mol	Chain	Res	Type
1	M	147	VAL
1	M	149	THR
1	M	155	LEU
1	M	156	LYS
1	M	163	LYS
1	M	178	LEU
1	M	189	SER
1	M	193	GLU
1	M	194	LEU
1	M	200	GLN
1	M	203	ARG
1	M	208	THR
1	M	210	LEU
1	M	211	GLU
1	M	220	GLU
1	M	221	LYS
1	M	228	GLU
1	M	233	LYS
1	M	234	LEU
1	M	248	LEU
1	M	249	ILE
1	M	257	ILE
1	M	258	ASP
1	M	260	GLN
1	M	262	GLU
1	M	263	THR
1	M	265	THR
1	M	266	GLU
1	M	267	GLU
1	M	275	LEU
1	M	277	SER
1	M	279	ASP
1	M	286	ASN
1	M	289	GLU
1	M	293	GLU
1	M	296	GLU
1	M	297	ASP
1	M	298	MET
1	M	305	ASP
1	M	309	GLU
1	M	312	LEU
1	N	11	ARG

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Mol	Chain	Res	Type
1	N	29	MET
1	N	32	CYS
1	N	34	ASP
1	N	39	GLU
1	N	40	SER
1	N	41	GLU
1	N	51	SER
1	N	59	ILE
1	N	63	LEU
1	N	64	ASN
1	N	83	GLU
1	N	100	GLU
1	N	105	LEU
1	N	116	THR
1	N	117	LYS
1	N	119	LEU
1	N	121	GLU
1	N	123	ILE
1	N	134	ASP
1	N	143	ARG
1	N	147	VAL
1	N	149	THR
1	N	155	LEU
1	N	156	LYS
1	N	163	LYS
1	N	178	LEU
1	N	189	SER
1	N	193	GLU
1	N	194	LEU
1	N	200	GLN
1	N	203	ARG
1	N	208	THR
1	N	210	LEU
1	N	211	GLU
1	N	220	GLU
1	N	221	LYS
1	N	228	GLU
1	N	233	LYS
1	N	234	LEU
1	N	248	LEU
1	N	249	ILE
1	N	257	ILE

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Mol	Chain	Res	Type
1	N	258	ASP
1	N	260	GLN
1	N	262	GLU
1	N	263	THR
1	N	265	THR
1	N	266	GLU
1	N	267	GLU
1	N	275	LEU
1	N	277	SER
1	N	279	ASP
1	N	286	ASN
1	N	289	GLU
1	N	293	GLU
1	N	296	GLU
1	N	297	ASP
1	N	298	MET
1	N	305	ASP
1	N	309	GLU
1	N	312	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	GLN
1	A	200	GLN
1	B	200	GLN
1	G	200	GLN
1	K	150	GLN
1	L	200	GLN
1	M	150	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

14 ligands are modelled in this entry.

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
4	ATP	M	401	-	26,33,33	0.92	1 (3%)	31,52,52	1.69	5 (16%)
4	ATP	K	401	-	26,33,33	0.92	1 (3%)	31,52,52	1.69	5 (16%)
4	ATP	A	401	-	26,33,33	0.93	1 (3%)	31,52,52	1.69	5 (16%)
4	ATP	L	401	-	26,33,33	0.92	1 (3%)	31,52,52	1.69	5 (16%)
4	ATP	J	401	-	26,33,33	0.93	1 (3%)	31,52,52	1.69	5 (16%)
4	ATP	F	401	-	26,33,33	0.93	1 (3%)	31,52,52	1.69	5 (16%)
4	ATP	B	401	-	26,33,33	0.93	1 (3%)	31,52,52	1.69	5 (16%)
4	ATP	D	401	-	26,33,33	0.93	1 (3%)	31,52,52	1.69	5 (16%)
4	ATP	H	401	-	26,33,33	0.93	1 (3%)	31,52,52	1.69	5 (16%)
4	ATP	N	401	-	26,33,33	0.92	1 (3%)	31,52,52	1.69	5 (16%)
4	ATP	E	401	-	26,33,33	0.93	1 (3%)	31,52,52	1.69	5 (16%)
4	ATP	I	401	-	26,33,33	0.92	1 (3%)	31,52,52	1.69	5 (16%)
4	ATP	G	401	-	26,33,33	0.93	1 (3%)	31,52,52	1.69	5 (16%)
4	ATP	C	401	-	26,33,33	0.92	1 (3%)	31,52,52	1.69	5 (16%)

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
4	ATP	M	401	-	-	0/18/38/38	0/3/3/3
4	ATP	K	401	-	-	0/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	A	401	-	-	0/18/38/38	0/3/3/3
4	ATP	L	401	-	-	0/18/38/38	0/3/3/3
4	ATP	J	401	-	-	0/18/38/38	0/3/3/3
4	ATP	F	401	-	-	0/18/38/38	0/3/3/3
4	ATP	B	401	-	-	0/18/38/38	0/3/3/3
4	ATP	D	401	-	-	0/18/38/38	0/3/3/3
4	ATP	H	401	-	-	0/18/38/38	0/3/3/3
4	ATP	N	401	-	-	0/18/38/38	0/3/3/3
4	ATP	E	401	-	-	0/18/38/38	0/3/3/3
4	ATP	I	401	-	-	0/18/38/38	0/3/3/3
4	ATP	G	401	-	-	0/18/38/38	0/3/3/3
4	ATP	C	401	-	-	0/18/38/38	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	401	ATP	C5-C4	2.34	1.47	1.40
4	H	401	ATP	C5-C4	2.34	1.47	1.40
4	I	401	ATP	C5-C4	2.34	1.47	1.40
4	G	401	ATP	C5-C4	2.33	1.47	1.40
4	J	401	ATP	C5-C4	2.33	1.47	1.40
4	K	401	ATP	C5-C4	2.33	1.47	1.40
4	C	401	ATP	C5-C4	2.33	1.47	1.40
4	E	401	ATP	C5-C4	2.32	1.47	1.40
4	L	401	ATP	C5-C4	2.32	1.47	1.40
4	M	401	ATP	C5-C4	2.32	1.47	1.40
4	F	401	ATP	C5-C4	2.32	1.47	1.40
4	D	401	ATP	C5-C4	2.32	1.47	1.40
4	B	401	ATP	C5-C4	2.31	1.47	1.40
4	N	401	ATP	C5-C4	2.30	1.47	1.40

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	401	ATP	PA-O3A-PB	-4.59	117.08	132.83
4	N	401	ATP	PA-O3A-PB	-4.59	117.09	132.83
4	K	401	ATP	PA-O3A-PB	-4.58	117.10	132.83
4	E	401	ATP	PA-O3A-PB	-4.58	117.10	132.83
4	H	401	ATP	PA-O3A-PB	-4.58	117.10	132.83
4	I	401	ATP	PA-O3A-PB	-4.58	117.10	132.83
4	J	401	ATP	PA-O3A-PB	-4.58	117.11	132.83
4	G	401	ATP	PA-O3A-PB	-4.58	117.11	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	401	ATP	PA-O3A-PB	-4.58	117.12	132.83
4	M	401	ATP	PA-O3A-PB	-4.58	117.12	132.83
4	D	401	ATP	PA-O3A-PB	-4.58	117.12	132.83
4	A	401	ATP	PA-O3A-PB	-4.58	117.12	132.83
4	B	401	ATP	PA-O3A-PB	-4.57	117.14	132.83
4	F	401	ATP	PA-O3A-PB	-4.57	117.14	132.83
4	A	401	ATP	PB-O3B-PG	-4.32	118.01	132.83
4	M	401	ATP	PB-O3B-PG	-4.32	118.01	132.83
4	L	401	ATP	PB-O3B-PG	-4.31	118.03	132.83
4	K	401	ATP	PB-O3B-PG	-4.31	118.03	132.83
4	H	401	ATP	PB-O3B-PG	-4.31	118.04	132.83
4	I	401	ATP	PB-O3B-PG	-4.31	118.05	132.83
4	J	401	ATP	PB-O3B-PG	-4.30	118.06	132.83
4	G	401	ATP	PB-O3B-PG	-4.30	118.06	132.83
4	N	401	ATP	PB-O3B-PG	-4.30	118.06	132.83
4	E	401	ATP	PB-O3B-PG	-4.30	118.06	132.83
4	F	401	ATP	PB-O3B-PG	-4.30	118.06	132.83
4	C	401	ATP	PB-O3B-PG	-4.30	118.06	132.83
4	B	401	ATP	PB-O3B-PG	-4.30	118.06	132.83
4	D	401	ATP	PB-O3B-PG	-4.29	118.09	132.83
4	J	401	ATP	C3'-C2'-C1'	3.27	105.90	100.98
4	M	401	ATP	C3'-C2'-C1'	3.27	105.90	100.98
4	B	401	ATP	C3'-C2'-C1'	3.26	105.89	100.98
4	F	401	ATP	C3'-C2'-C1'	3.26	105.89	100.98
4	K	401	ATP	C3'-C2'-C1'	3.26	105.88	100.98
4	D	401	ATP	C3'-C2'-C1'	3.25	105.88	100.98
4	A	401	ATP	C3'-C2'-C1'	3.25	105.87	100.98
4	I	401	ATP	C3'-C2'-C1'	3.25	105.87	100.98
4	G	401	ATP	C3'-C2'-C1'	3.25	105.86	100.98
4	N	401	ATP	C3'-C2'-C1'	3.24	105.86	100.98
4	H	401	ATP	C3'-C2'-C1'	3.24	105.86	100.98
4	C	401	ATP	C3'-C2'-C1'	3.24	105.86	100.98
4	E	401	ATP	C3'-C2'-C1'	3.24	105.86	100.98
4	L	401	ATP	C3'-C2'-C1'	3.24	105.85	100.98
4	G	401	ATP	N3-C2-N1	-3.09	123.86	128.68
4	B	401	ATP	N3-C2-N1	-3.08	123.86	128.68
4	A	401	ATP	N3-C2-N1	-3.08	123.86	128.68
4	K	401	ATP	N3-C2-N1	-3.07	123.88	128.68
4	L	401	ATP	N3-C2-N1	-3.07	123.88	128.68
4	D	401	ATP	N3-C2-N1	-3.06	123.89	128.68
4	N	401	ATP	N3-C2-N1	-3.06	123.90	128.68
4	E	401	ATP	N3-C2-N1	-3.06	123.90	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	401	ATP	N3-C2-N1	-3.05	123.90	128.68
4	F	401	ATP	N3-C2-N1	-3.05	123.91	128.68
4	C	401	ATP	N3-C2-N1	-3.05	123.92	128.68
4	M	401	ATP	N3-C2-N1	-3.04	123.92	128.68
4	H	401	ATP	N3-C2-N1	-3.02	123.95	128.68
4	J	401	ATP	N3-C2-N1	-3.02	123.96	128.68
4	I	401	ATP	C4-C5-N7	-2.38	106.92	109.40
4	C	401	ATP	C4-C5-N7	-2.37	106.93	109.40
4	K	401	ATP	C4-C5-N7	-2.36	106.94	109.40
4	F	401	ATP	C4-C5-N7	-2.36	106.94	109.40
4	A	401	ATP	C4-C5-N7	-2.36	106.94	109.40
4	G	401	ATP	C4-C5-N7	-2.35	106.94	109.40
4	D	401	ATP	C4-C5-N7	-2.35	106.95	109.40
4	B	401	ATP	C4-C5-N7	-2.34	106.96	109.40
4	N	401	ATP	C4-C5-N7	-2.34	106.96	109.40
4	H	401	ATP	C4-C5-N7	-2.34	106.96	109.40
4	J	401	ATP	C4-C5-N7	-2.34	106.96	109.40
4	L	401	ATP	C4-C5-N7	-2.33	106.97	109.40
4	E	401	ATP	C4-C5-N7	-2.32	106.98	109.40
4	M	401	ATP	C4-C5-N7	-2.32	106.98	109.40

There are no chirality outliers.

There are no torsion outliers.

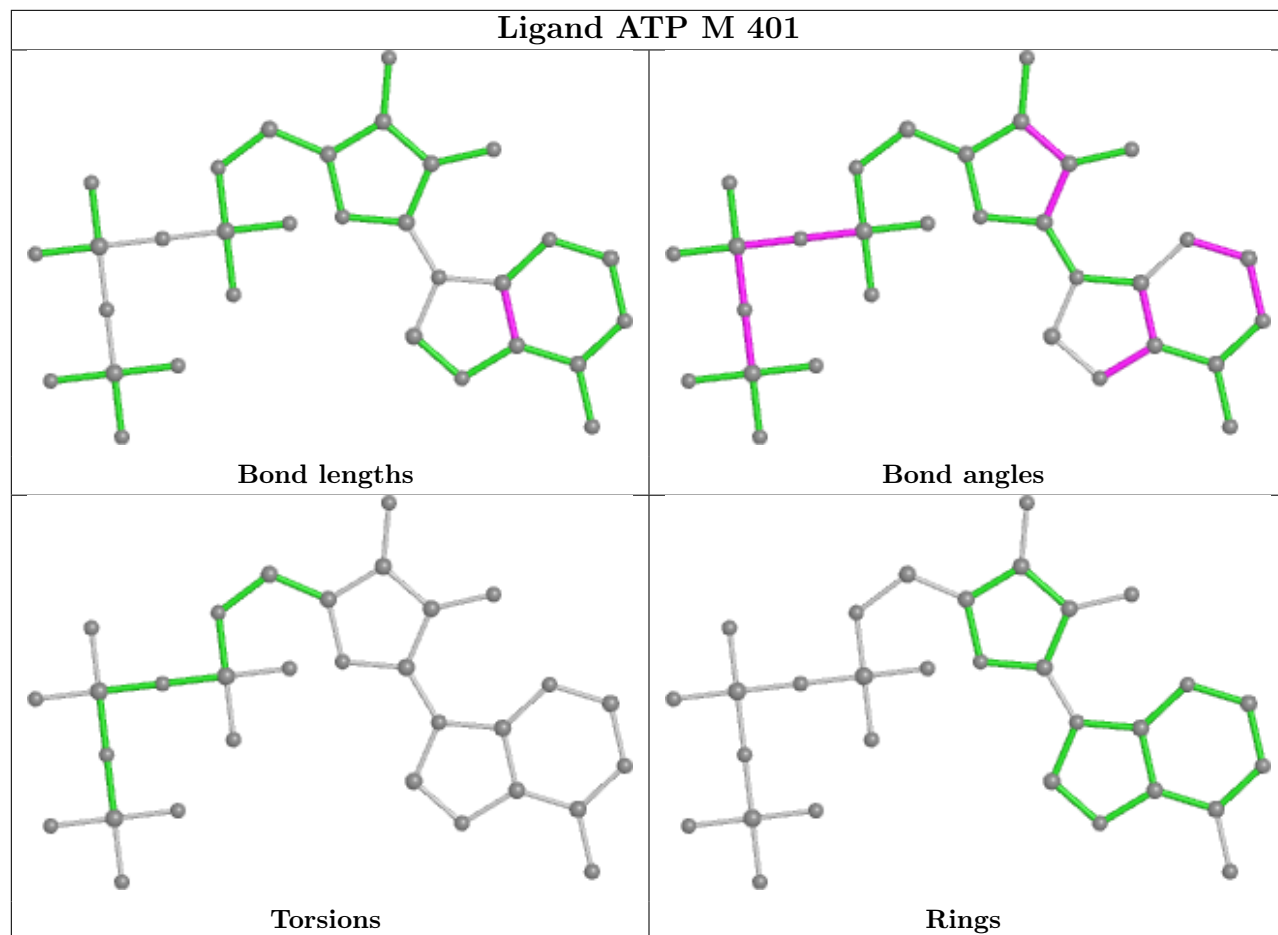
There are no ring outliers.

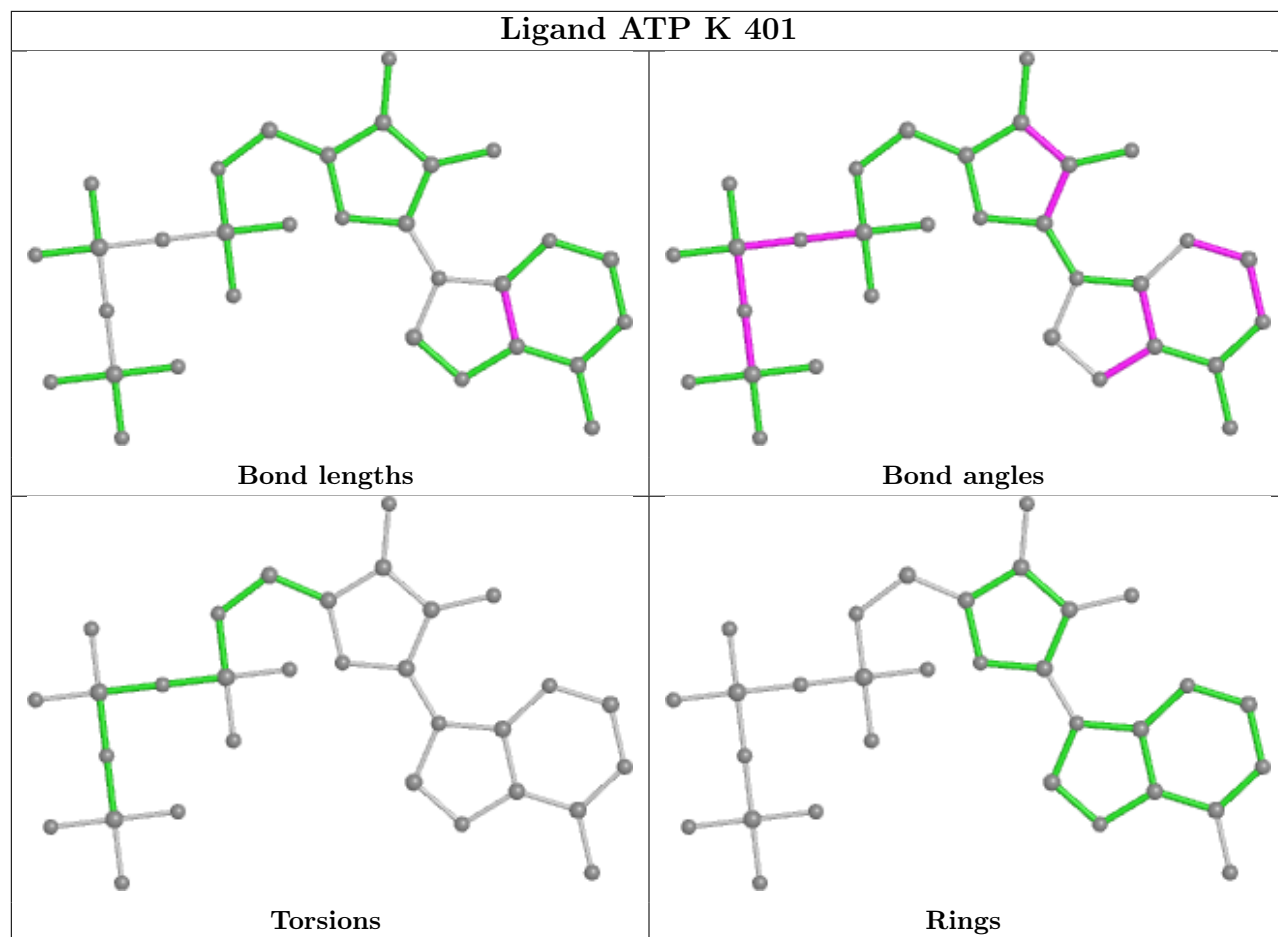
3 monomers are involved in 4 short contacts:

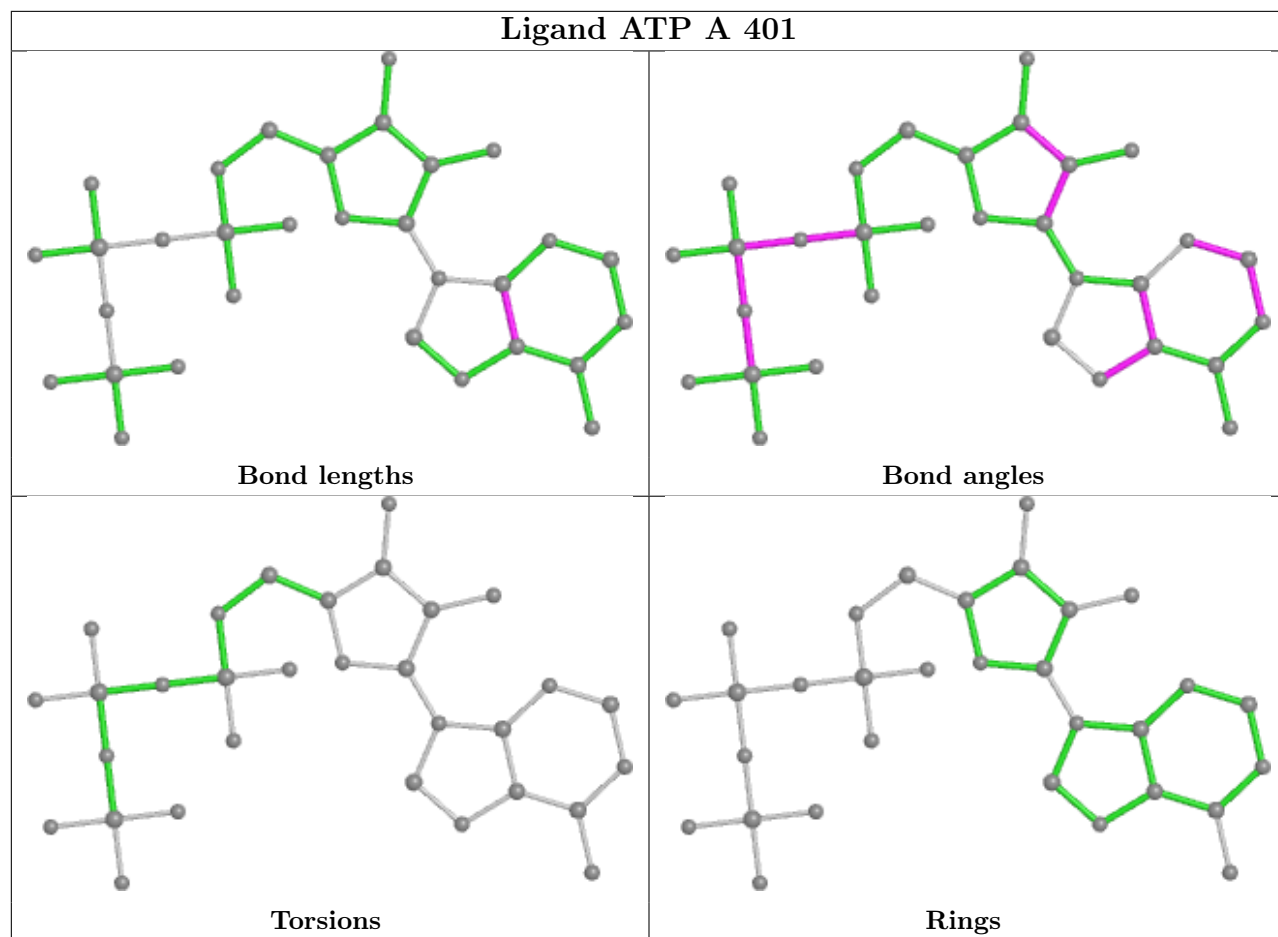
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	401	ATP	1	0
4	L	401	ATP	2	0
4	D	401	ATP	1	0

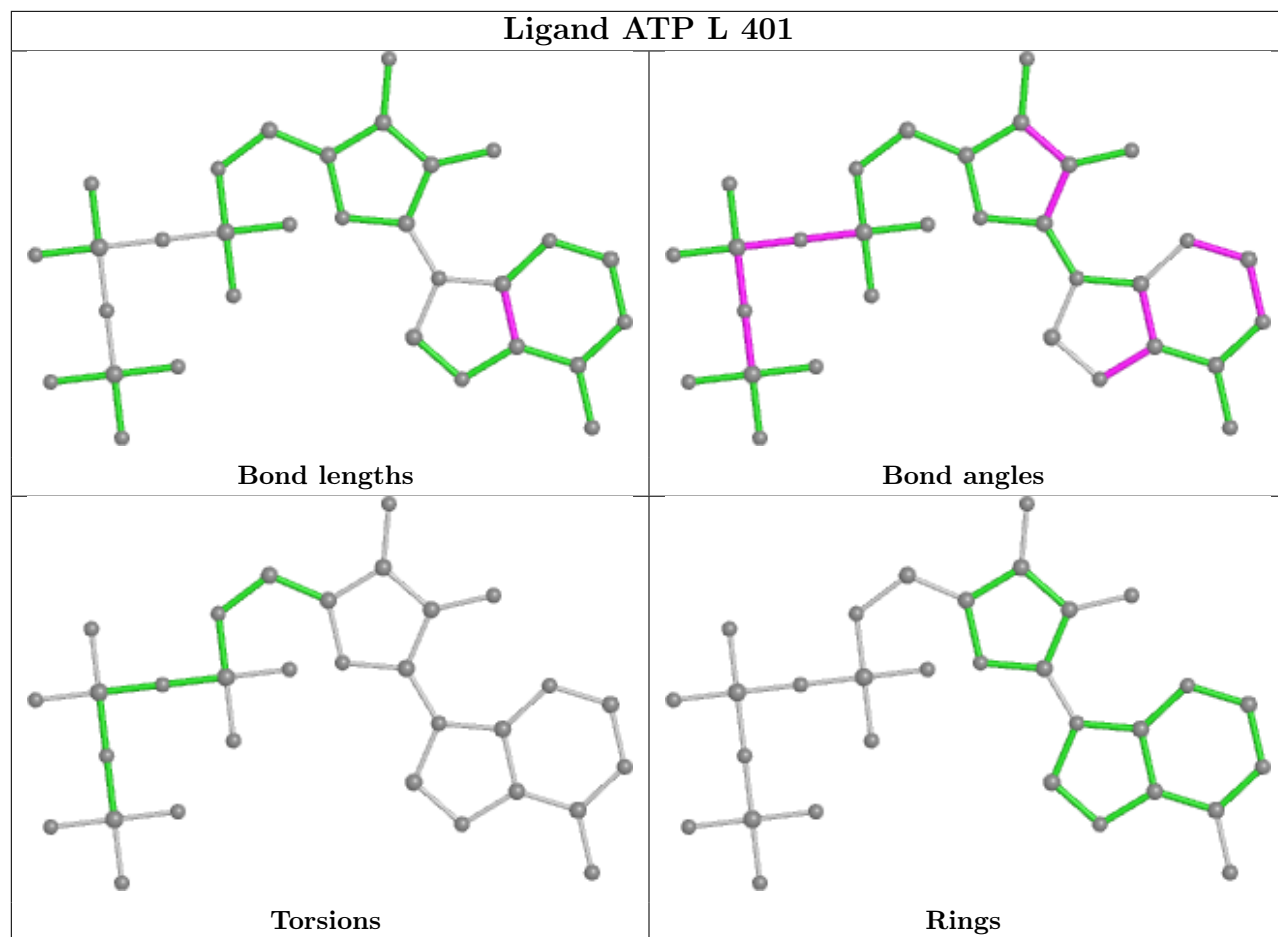
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

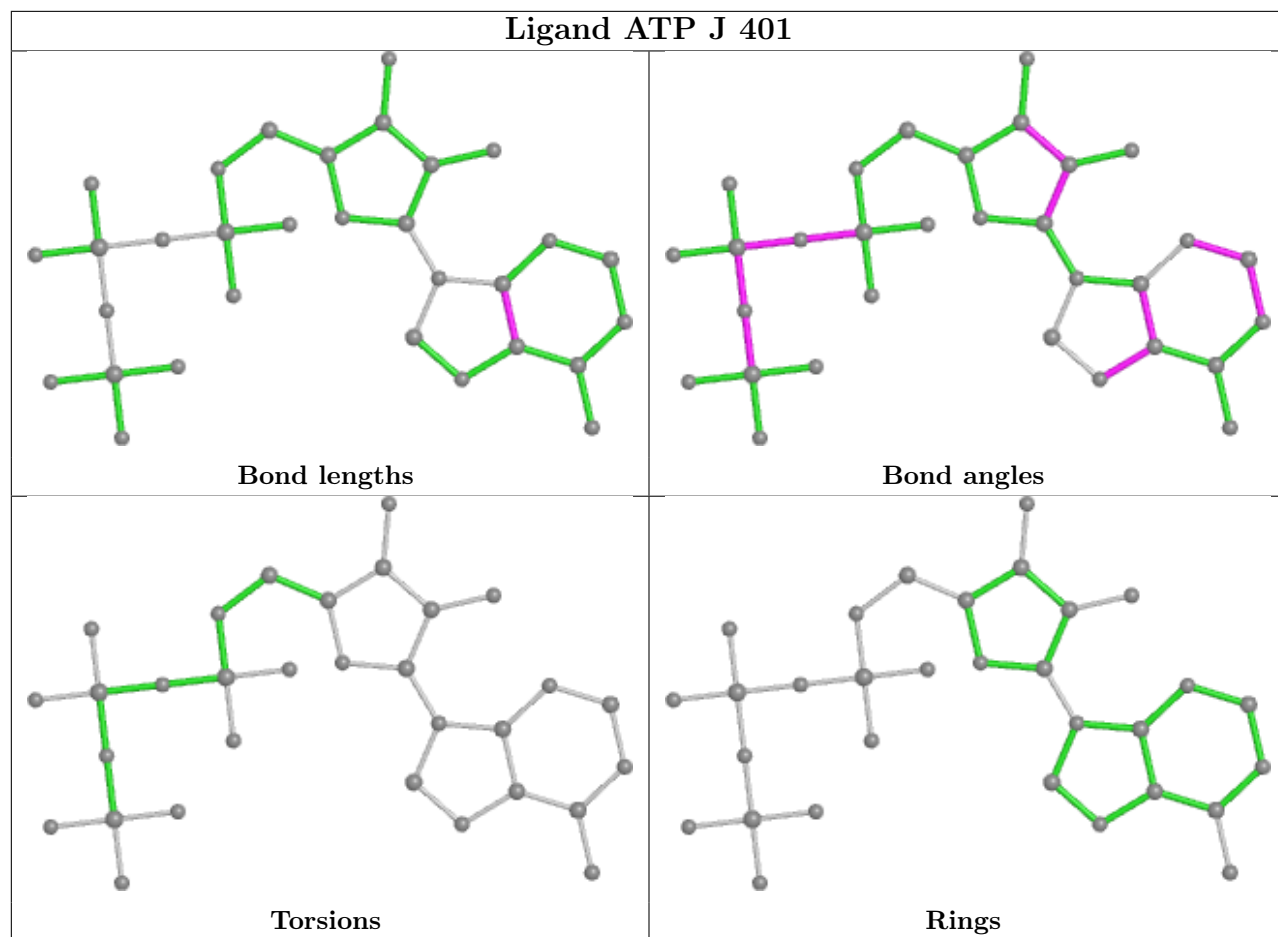
equivalents in the CSD to analyse the geometry.

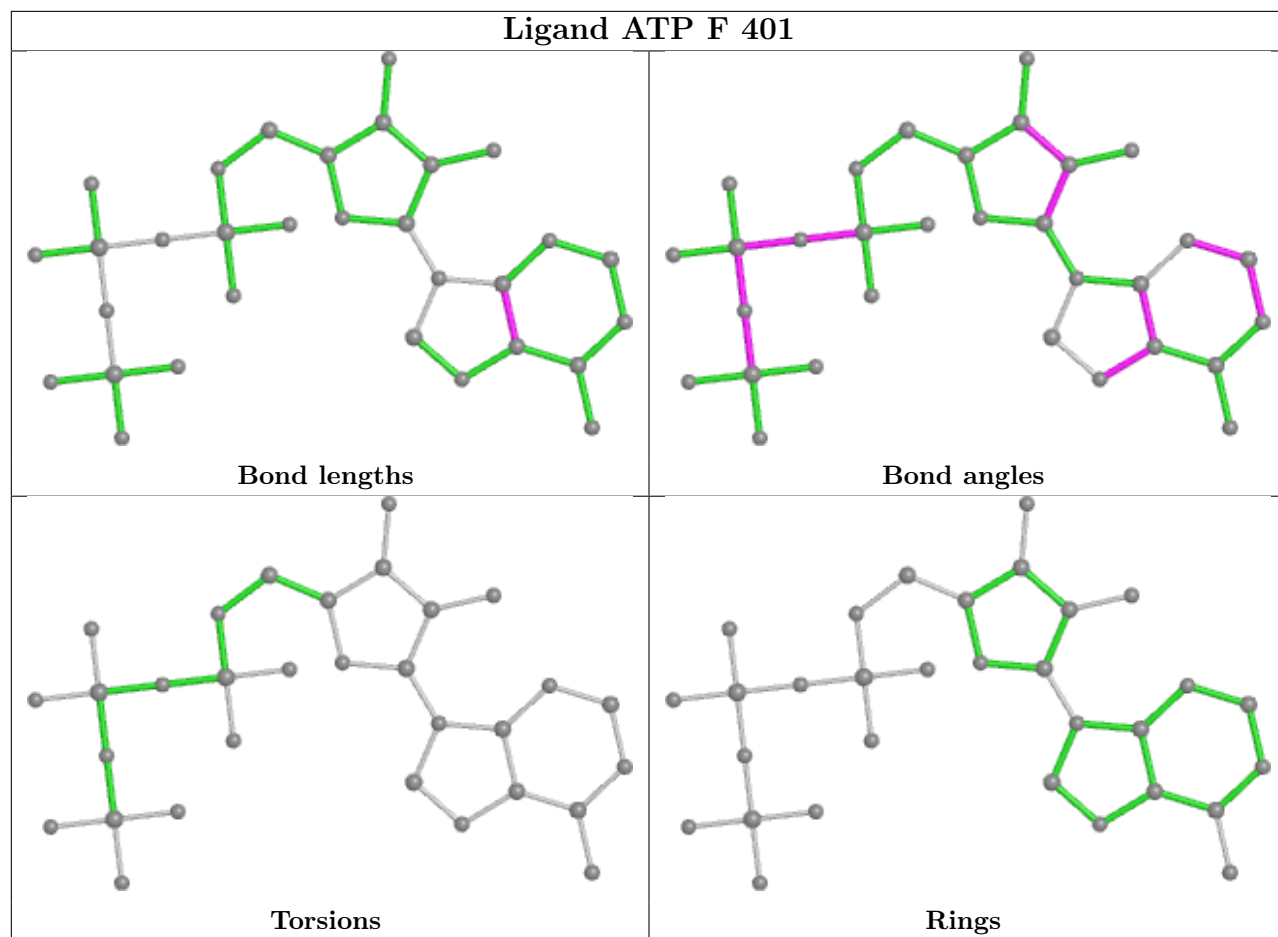


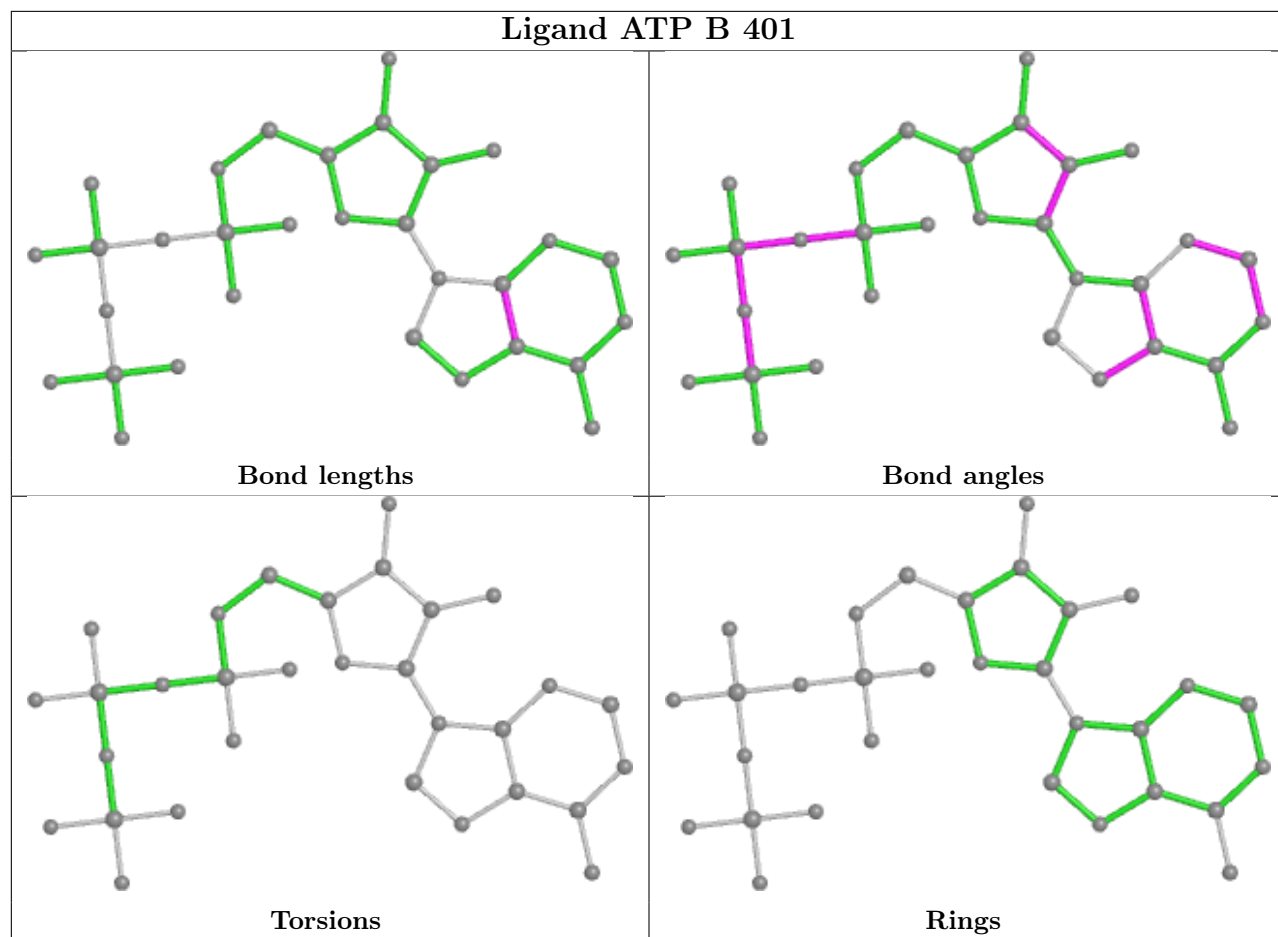


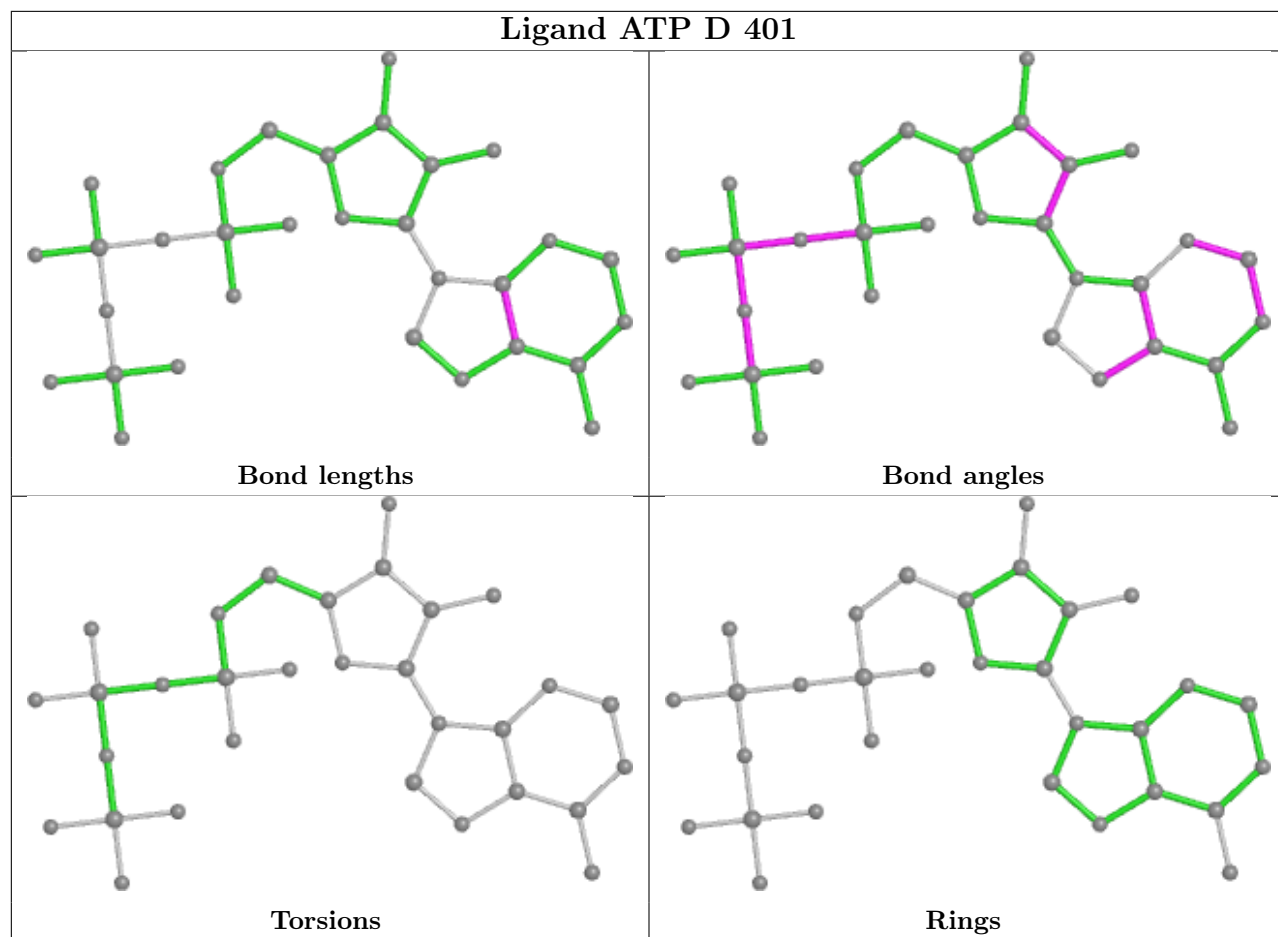


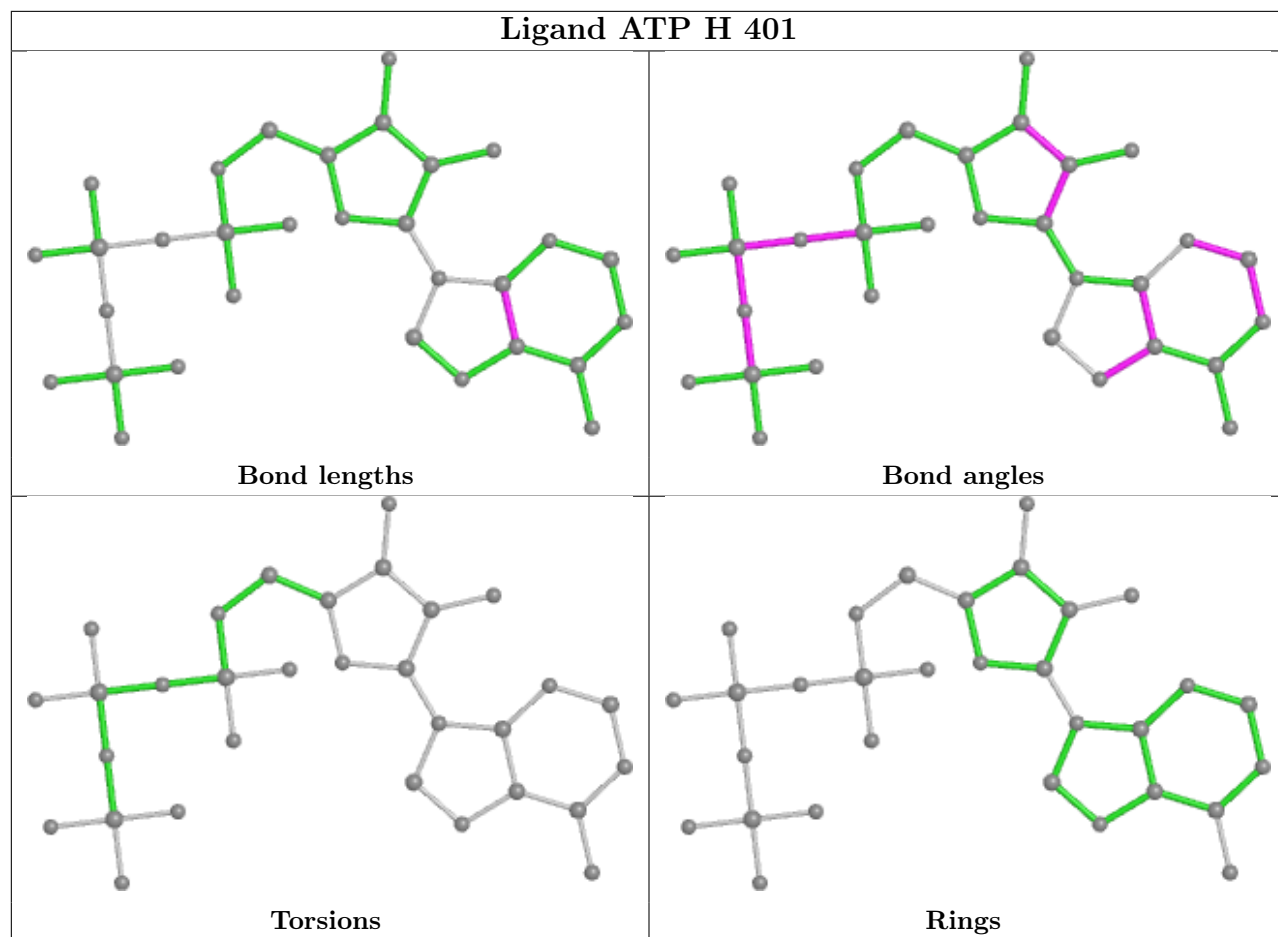


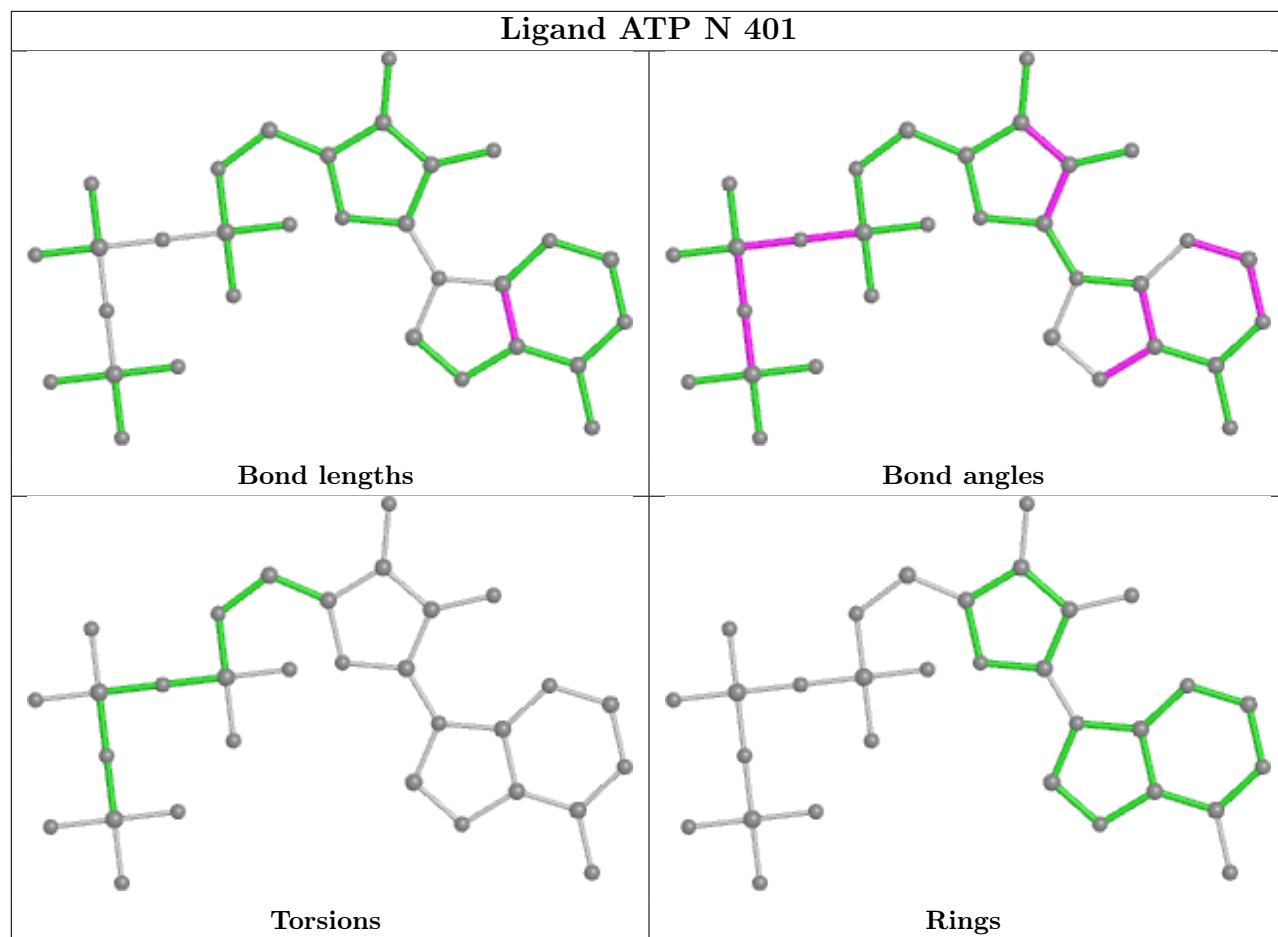


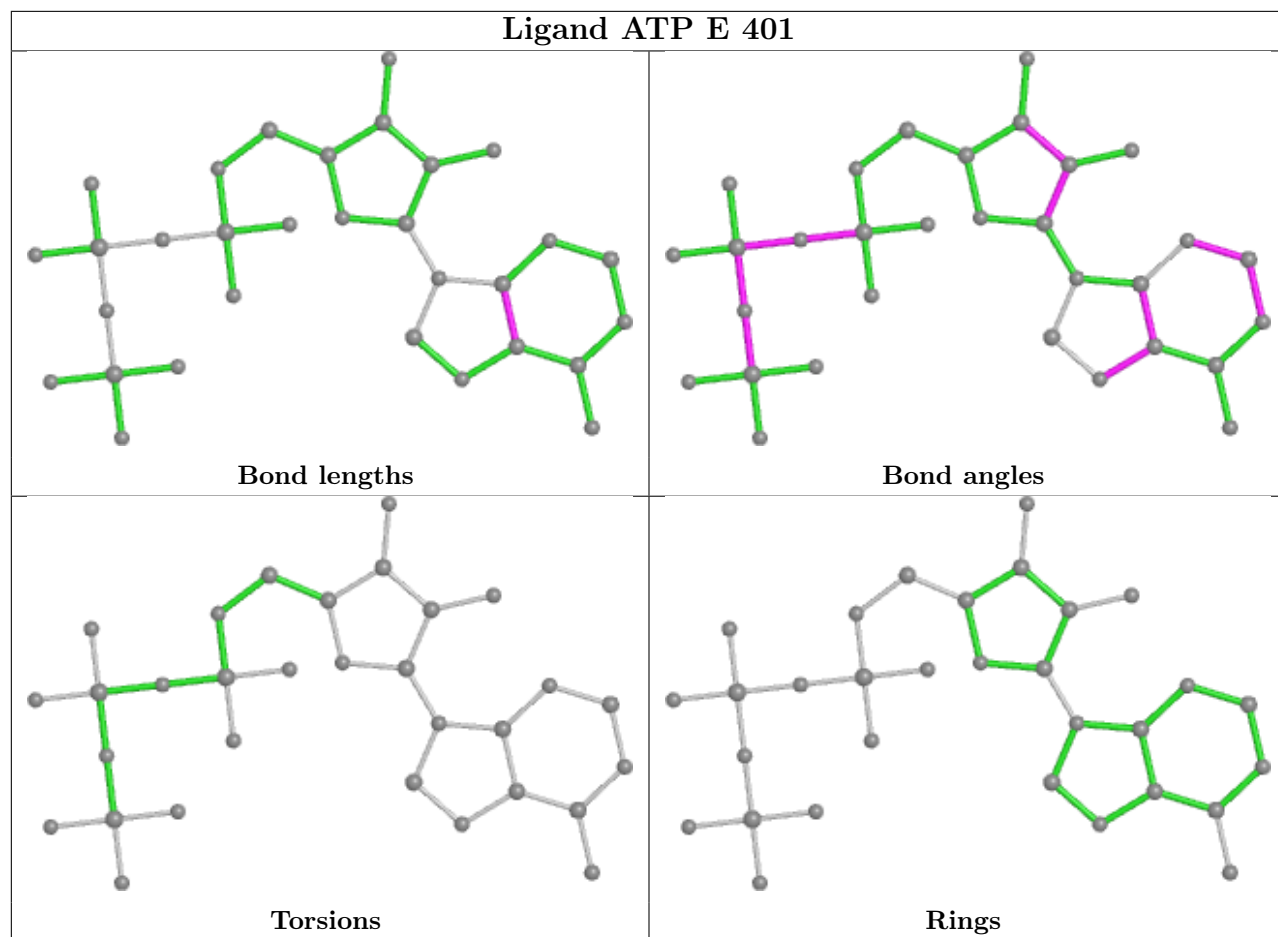


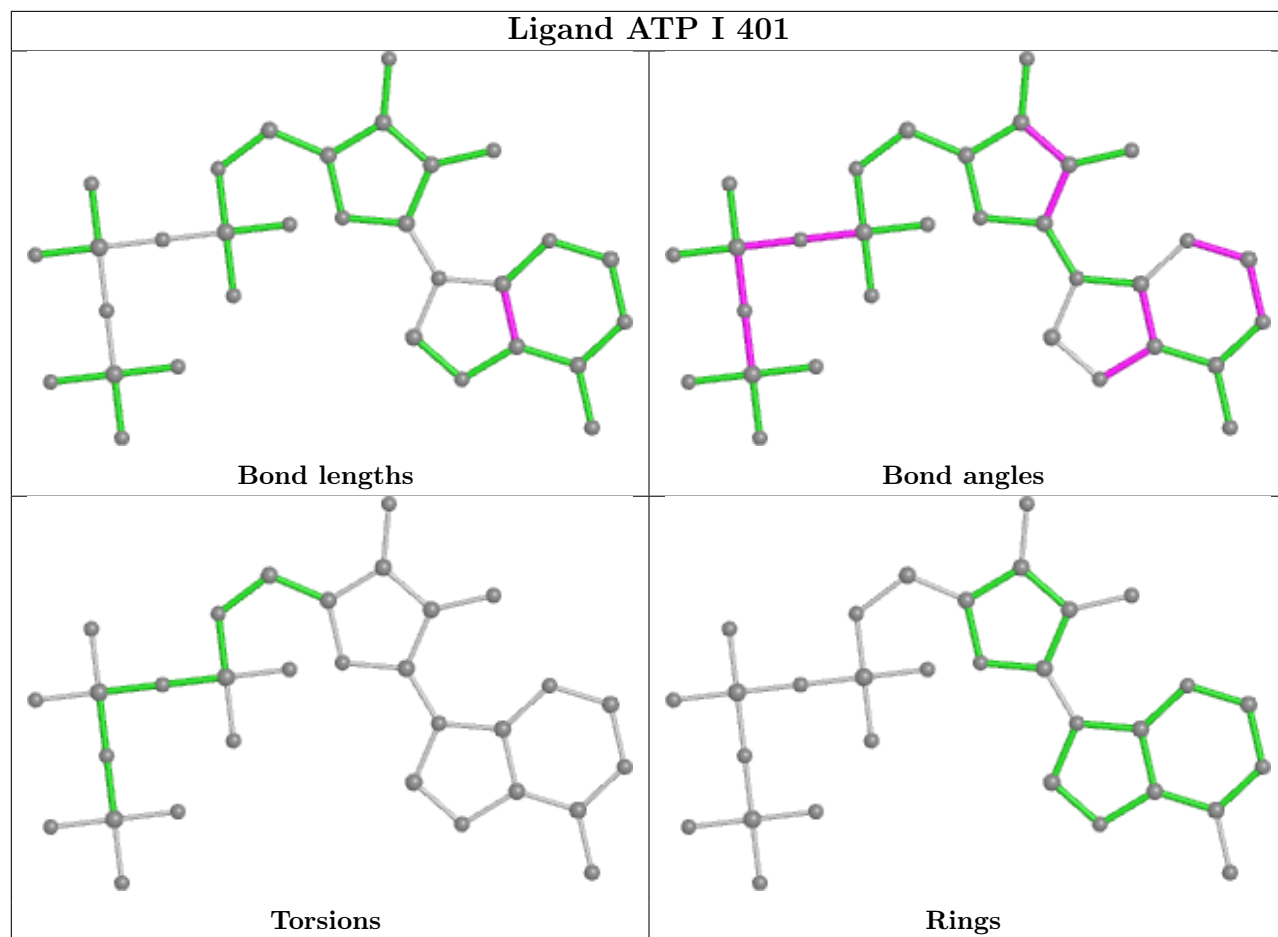


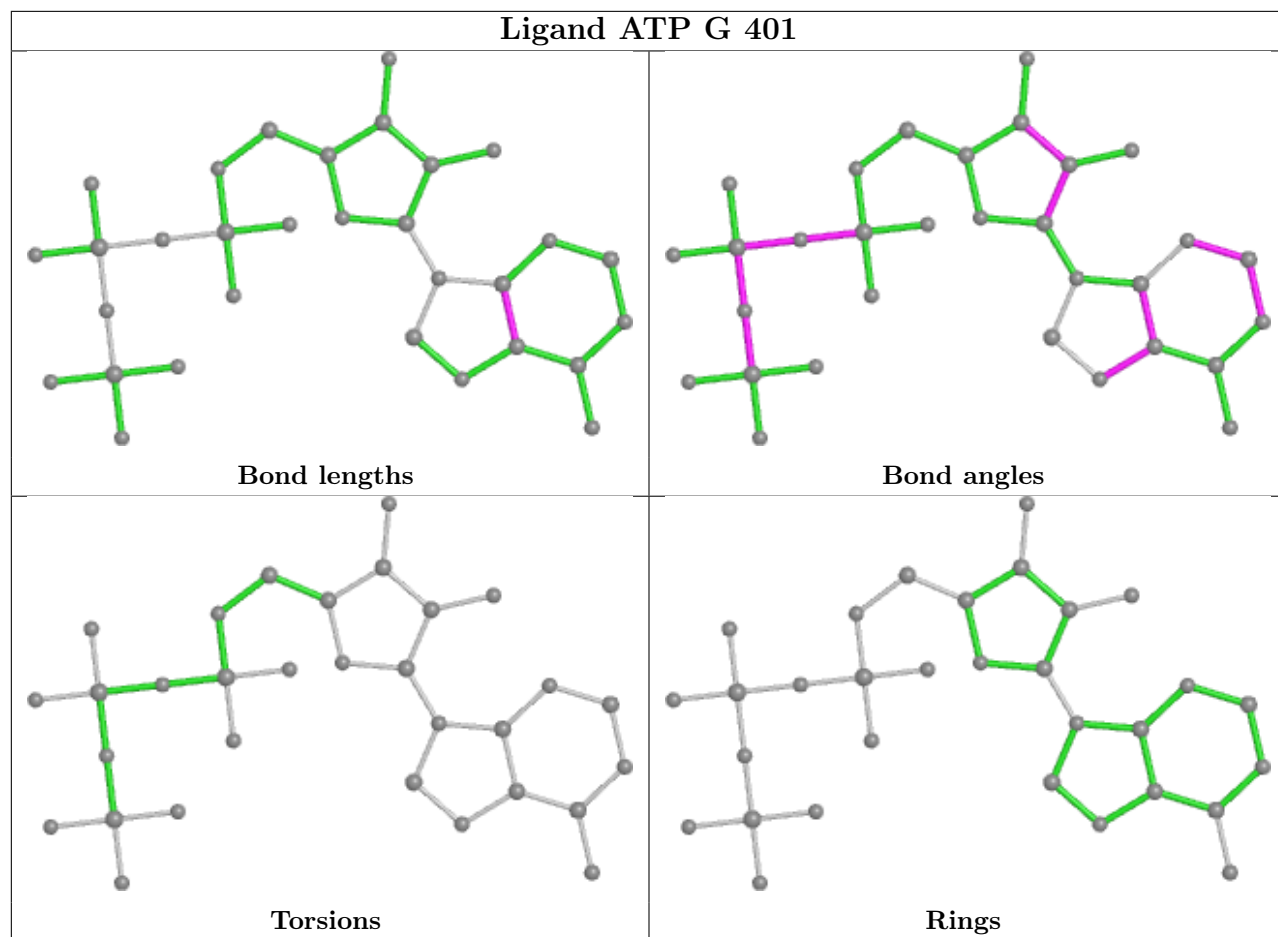


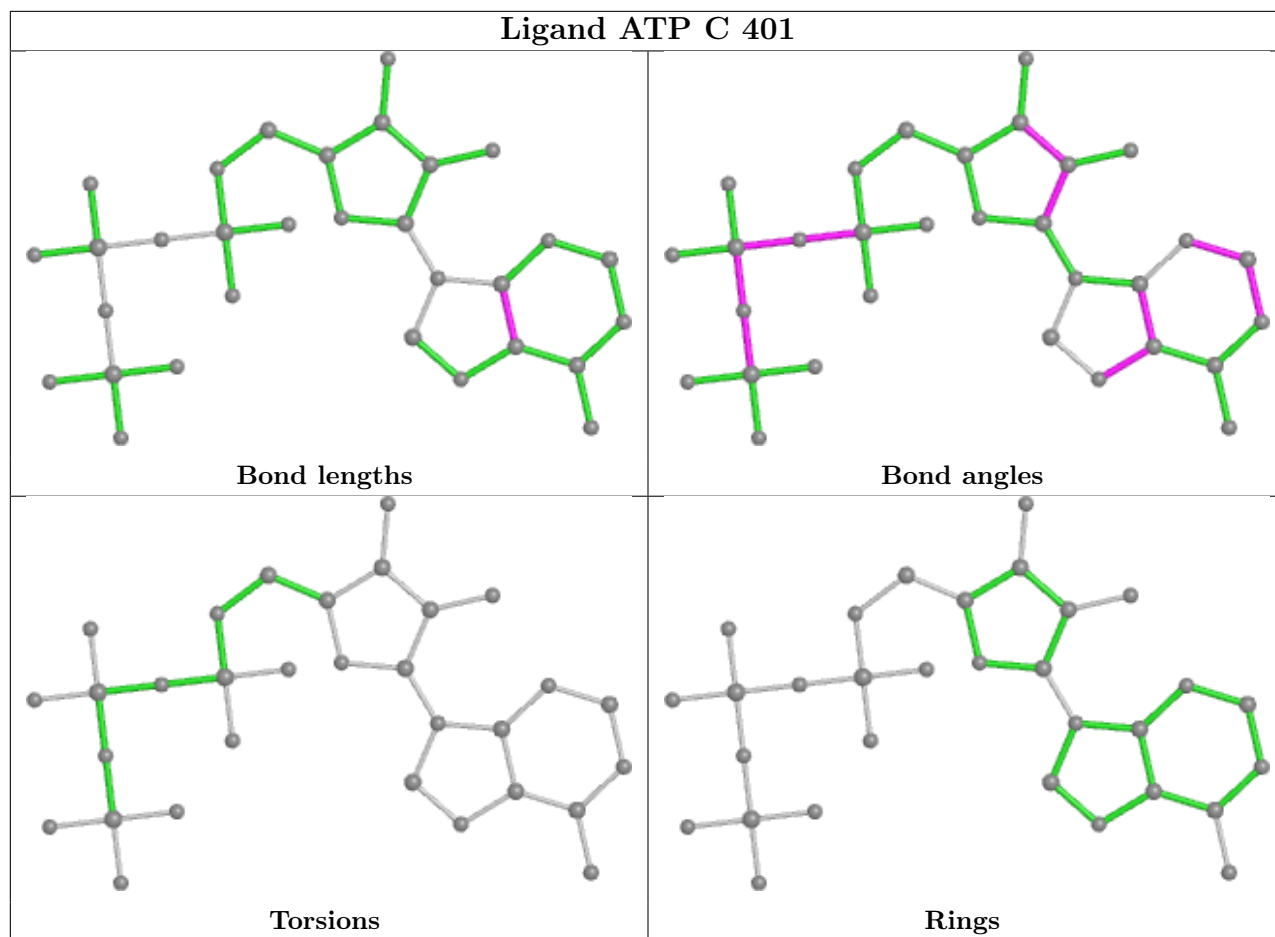












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	P	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	P	35:DG	O3'	36:DC	P	5.26
1	P	20:DG	O3'	21:DA	P	3.23

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-26477. 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

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal surface views

This section was not generated.

6.5 Mask visualisation

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

7 Map analysis

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

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.