



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 12:43 AM UTC

PDB ID : 6OIF / pdb_00006oif
EMDB ID : EMD-20076
Title : Cryo-EM structure of human TorsinA filament
Authors : Zheng, W.; Demircioglu, F.E.; Schwartz, T.U.; Egelman, E.H.
Deposited on : 2019-04-09
Resolution : 4.40 Å(reported)
Based on initial model : 5J1S

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 EMD 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

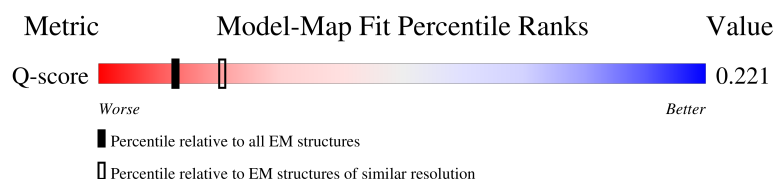
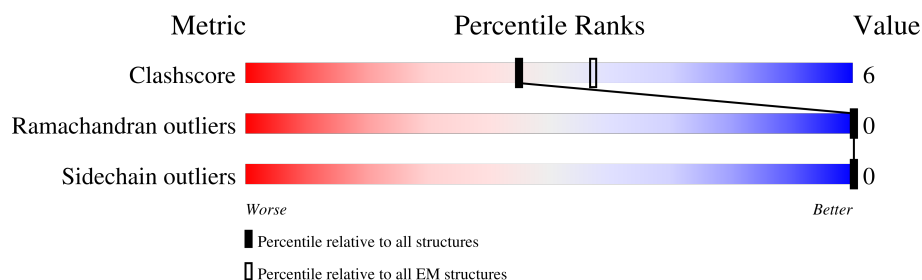
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 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	-
Q-score	-	25397	3132 (3.91 - 4.90)

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	A	282	28% 83% 17%
1	B	282	28% 82% 18%
1	C	282	29% 84% 16%
1	D	282	29% 82% 18%

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Mol	Chain	Length	Quality of chain		
1	E	282	31%	82%	18%
1	F	282	30%	82%	18%
1	G	282	32%	82%	18%
1	H	282	30%	82%	18%
1	I	282	32%	82%	18%
1	J	282	33%	82%	18%
1	K	282	31%	82%	18%
1	L	282	33%	83%	17%
1	M	282	33%	82%	18%
1	N	282	35%	82%	18%
1	O	282	34%	82%	18%
1	P	282	37%	82%	18%
1	Q	282	34%	83%	17%
1	R	282	40%	82%	18%
1	S	282	38%	83%	17%
1	T	282	41%	82%	18%
1	U	282	38%	82%	18%
1	V	282	47%	82%	18%
1	W	282	39%	82%	18%
1	X	282	48%	82%	18%
1	Y	282	42%	83%	17%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 115325 atoms, of which 57050 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 Torsin-1A.

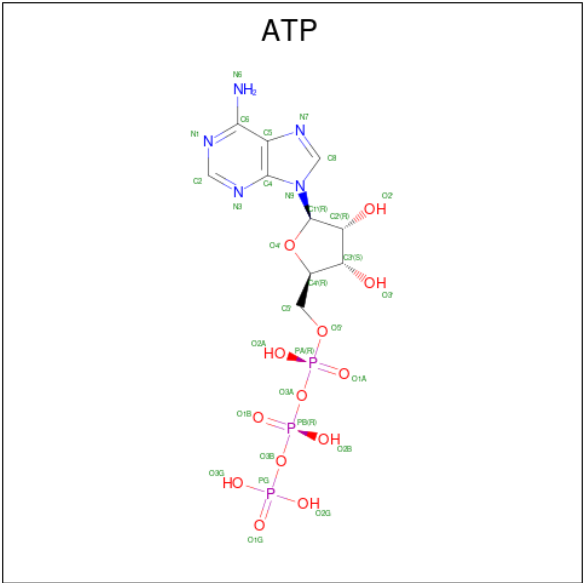
Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	282	Total	C	H	N	O	S	0	0
			4570	1485	2270	385	421	9		
1	B	282	Total	C	H	N	O	S	0	0
			4570	1485	2270	385	421	9		
1	C	282	Total	C	H	N	O	S	0	0
			4570	1485	2270	385	421	9		
1	D	282	Total	C	H	N	O	S	0	0
			4570	1485	2270	385	421	9		
1	E	282	Total	C	H	N	O	S	0	0
			4570	1485	2270	385	421	9		
1	F	282	Total	C	H	N	O	S	0	0
			4570	1485	2270	385	421	9		
1	G	282	Total	C	H	N	O	S	0	0
			4570	1485	2270	385	421	9		
1	H	282	Total	C	H	N	O	S	0	0
			4570	1485	2270	385	421	9		
1	I	282	Total	C	H	N	O	S	0	0
			4570	1485	2270	385	421	9		
1	J	282	Total	C	H	N	O	S	0	0
			4570	1485	2270	385	421	9		
1	K	282	Total	C	H	N	O	S	0	0
			4570	1485	2270	385	421	9		
1	L	282	Total	C	H	N	O	S	0	0
			4570	1485	2270	385	421	9		
1	M	282	Total	C	H	N	O	S	0	0
			4570	1485	2270	385	421	9		
1	N	282	Total	C	H	N	O	S	0	0
			4570	1485	2270	385	421	9		
1	O	282	Total	C	H	N	O	S	0	0
			4570	1485	2270	385	421	9		
1	P	282	Total	C	H	N	O	S	0	0
			4570	1485	2270	385	421	9		
1	Q	282	Total	C	H	N	O	S	0	0
			4570	1485	2270	385	421	9		

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Mol	Chain	Residues	Atoms						AltConf	Trace
1	R	282	Total 4570	C 1485	H 2270	N 385	O 421	S 9	0	0
1	S	282	Total 4570	C 1485	H 2270	N 385	O 421	S 9	0	0
1	T	282	Total 4570	C 1485	H 2270	N 385	O 421	S 9	0	0
1	U	282	Total 4570	C 1485	H 2270	N 385	O 421	S 9	0	0
1	V	282	Total 4570	C 1485	H 2270	N 385	O 421	S 9	0	0
1	W	282	Total 4570	C 1485	H 2270	N 385	O 421	S 9	0	0
1	X	282	Total 4570	C 1485	H 2270	N 385	O 421	S 9	0	0
1	Y	282	Total 4570	C 1485	H 2270	N 385	O 421	S 9	0	0

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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Mol	Chain	Residues	Atoms						AltConf
2	D	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
2	E	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
2	F	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
2	G	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
2	H	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
2	I	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
2	J	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
2	K	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
2	L	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
2	M	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
2	N	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
2	O	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
2	P	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
2	Q	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
2	R	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
2	S	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
2	T	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
2	U	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
2	V	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
2	W	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
2	X	1	Total 43	C 10	H 12	N 5	O 13	P 3	0

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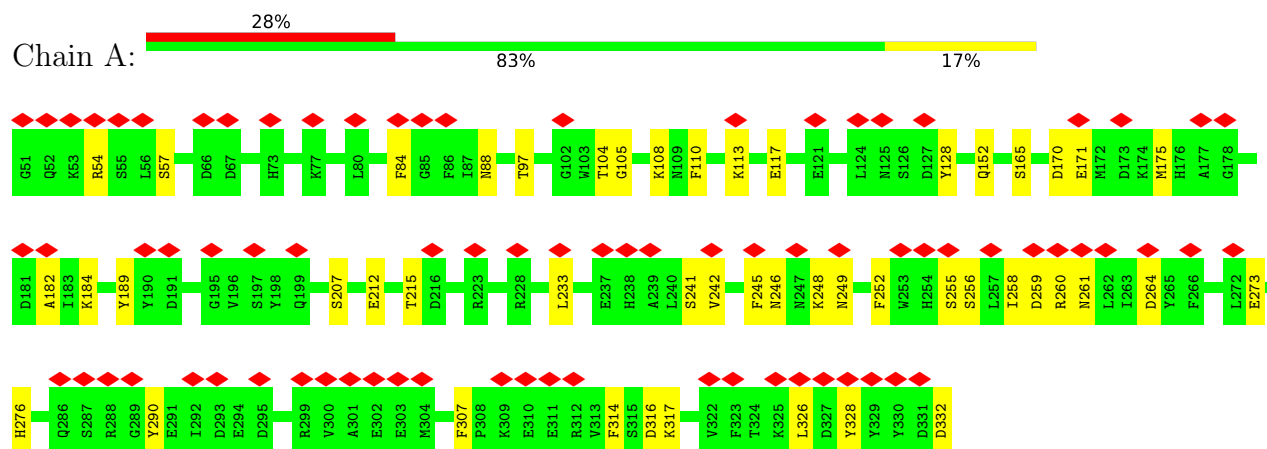
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Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
2	X	1	43	10	12	5	13	3	0

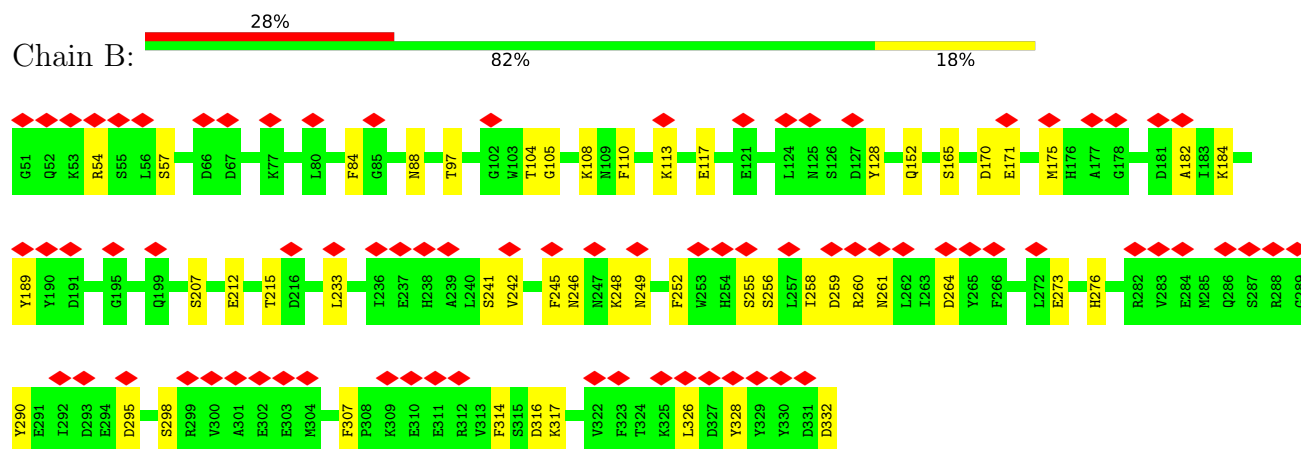
3 Residue-property plots [i](#)

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

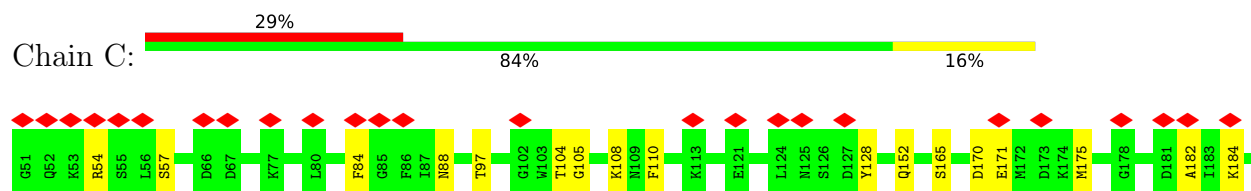
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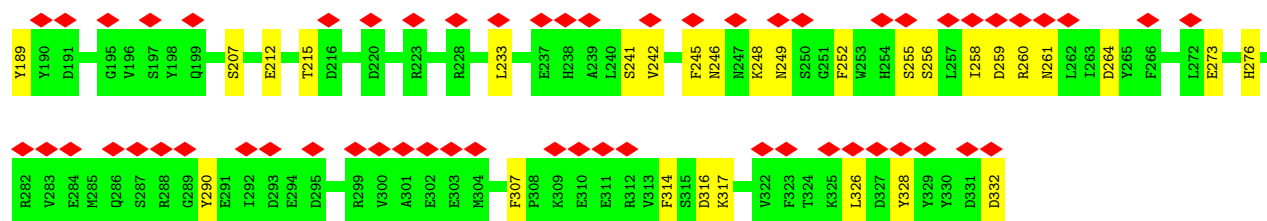


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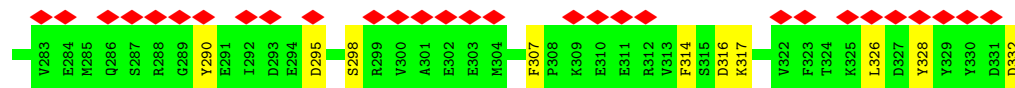
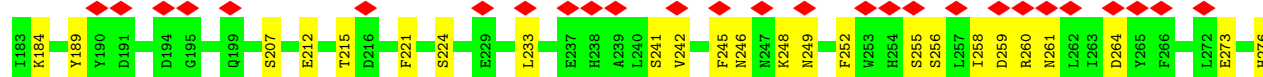
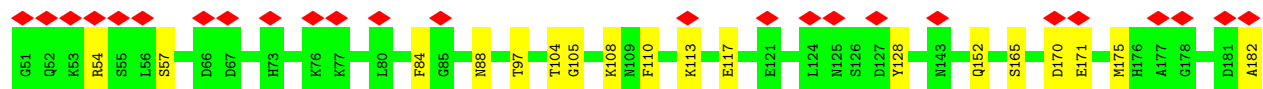
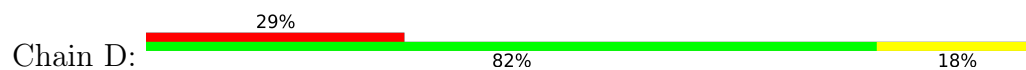


• Molecule 1: Torsin-1A

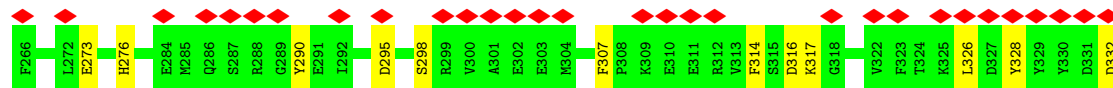
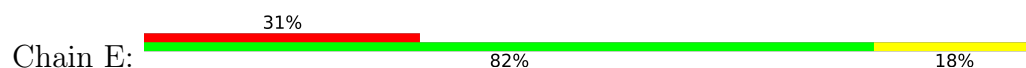




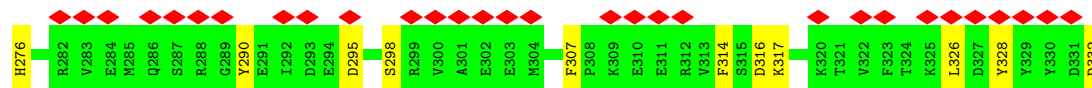
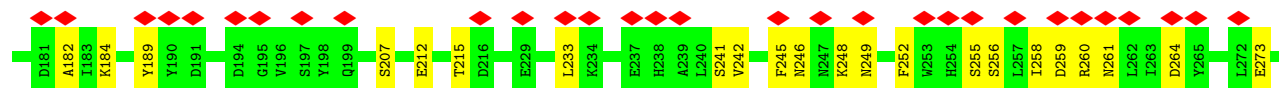
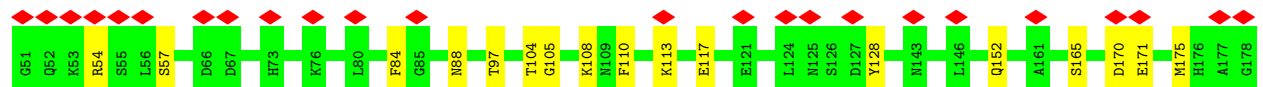
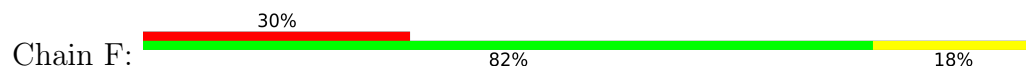
• Molecule 1: Torsin-1A



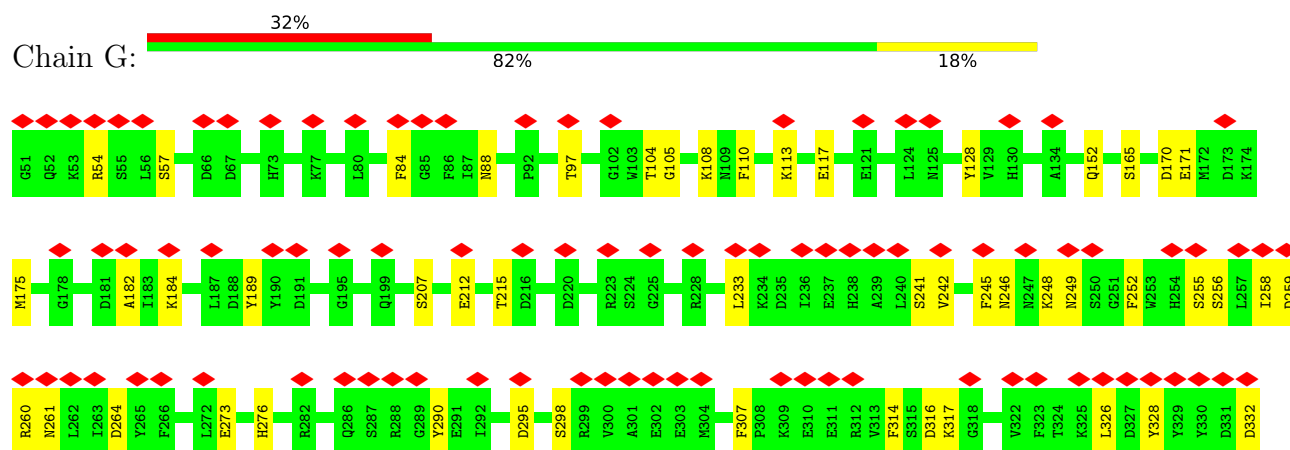
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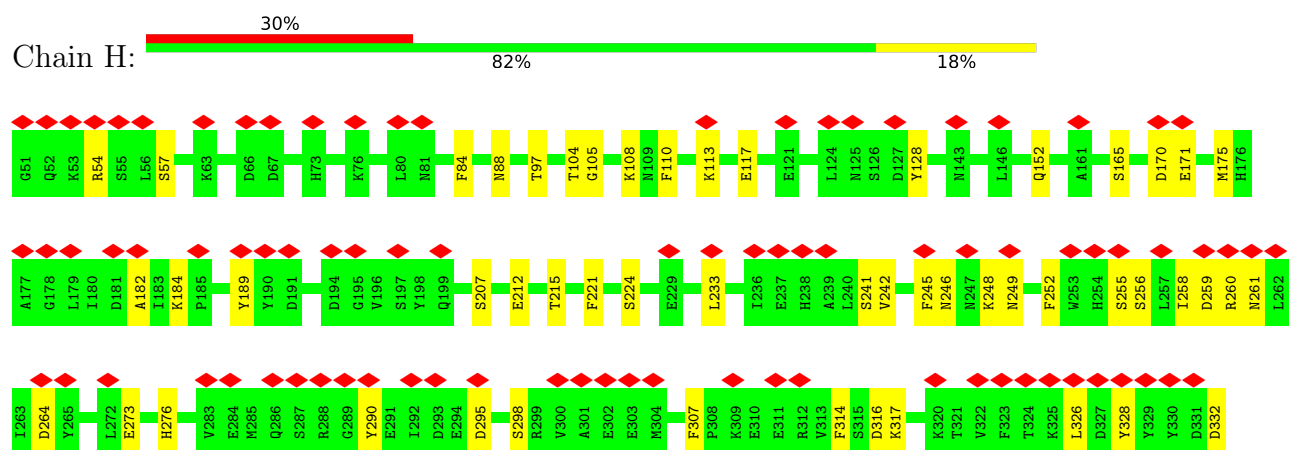
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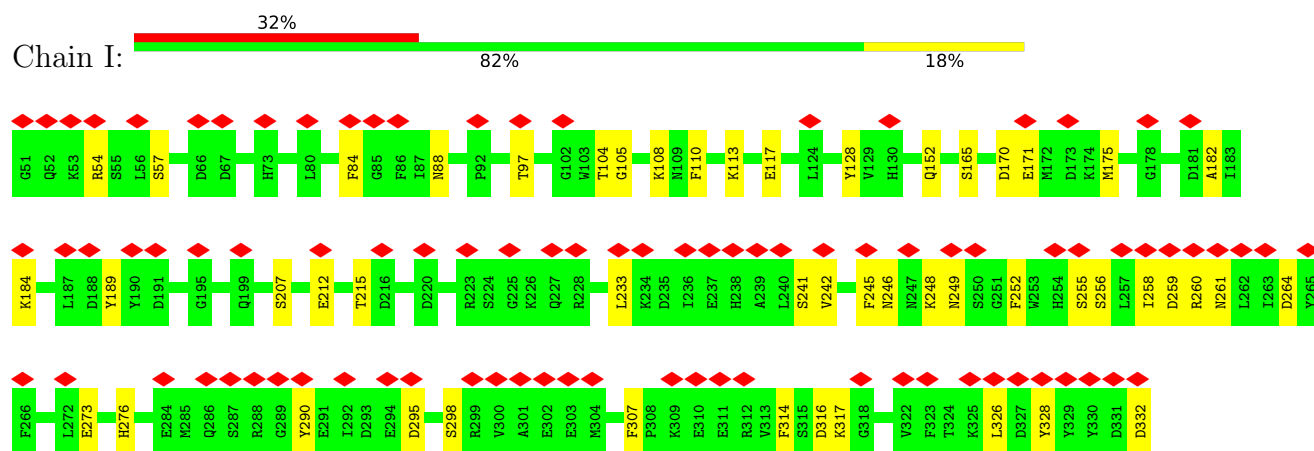
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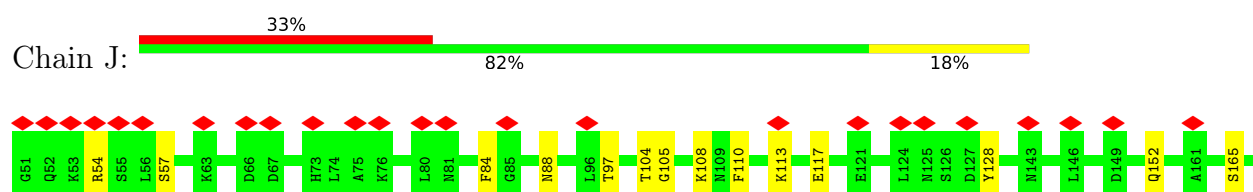
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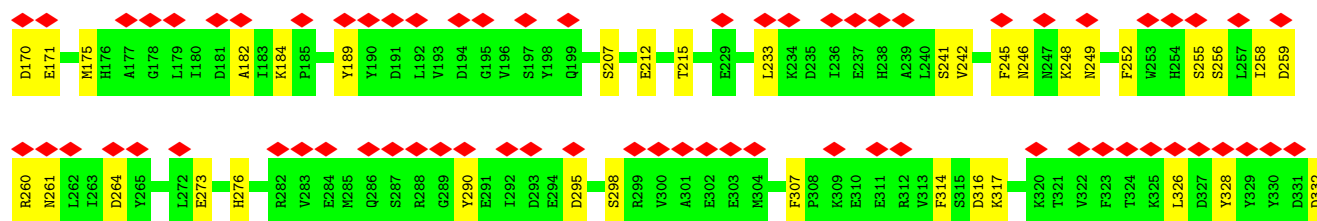


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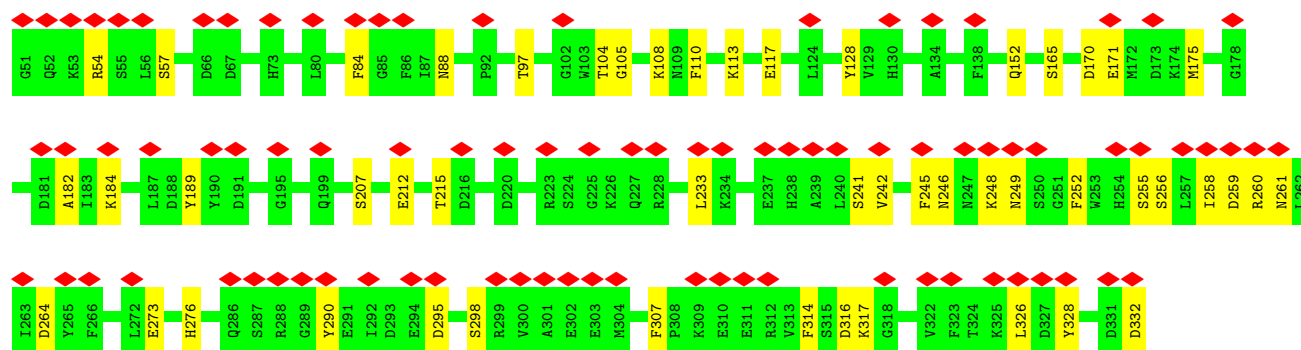
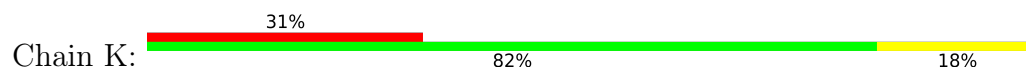


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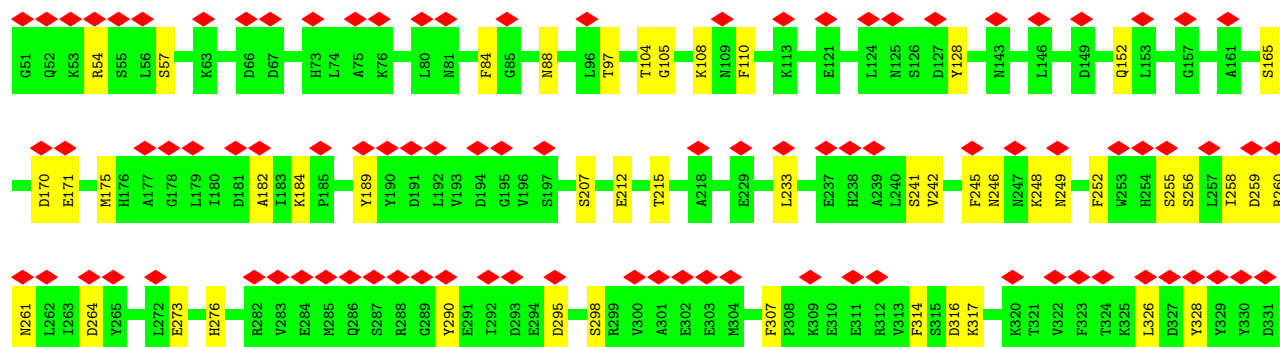
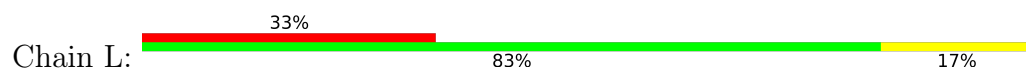




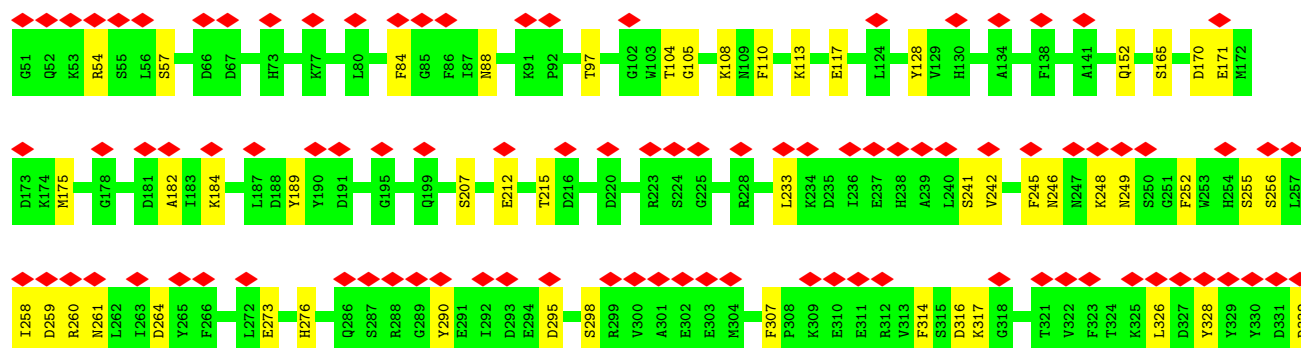
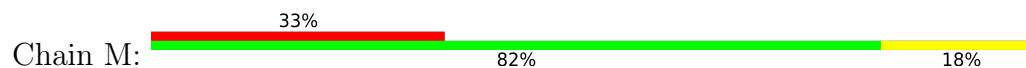
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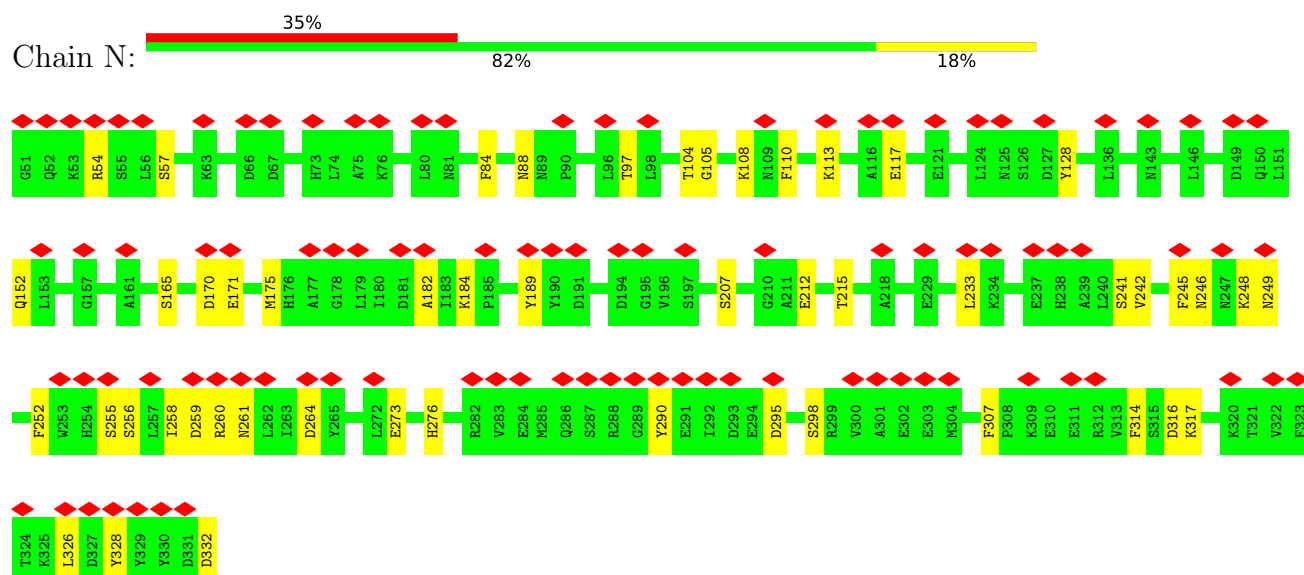
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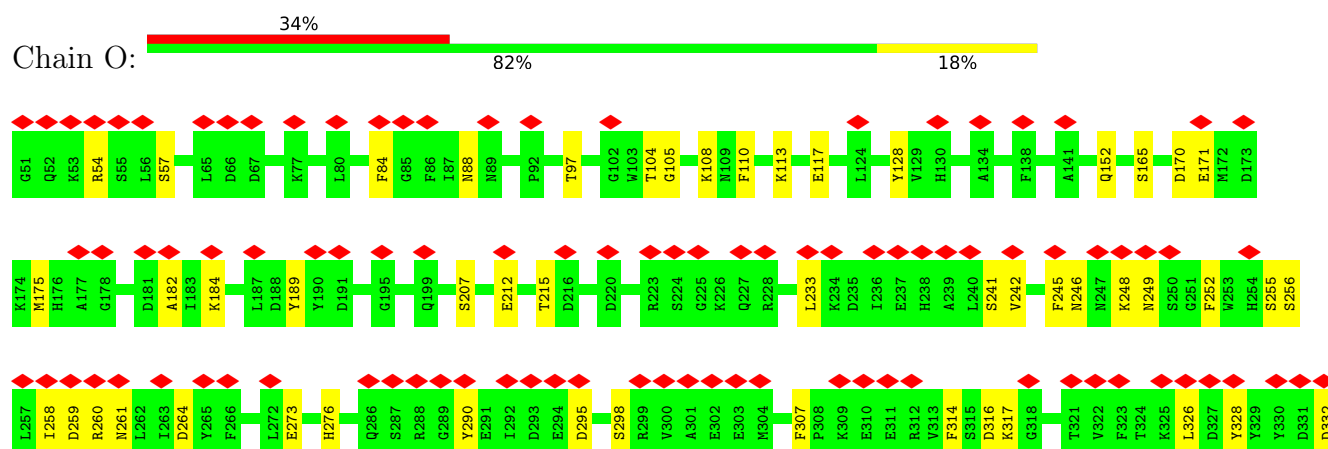
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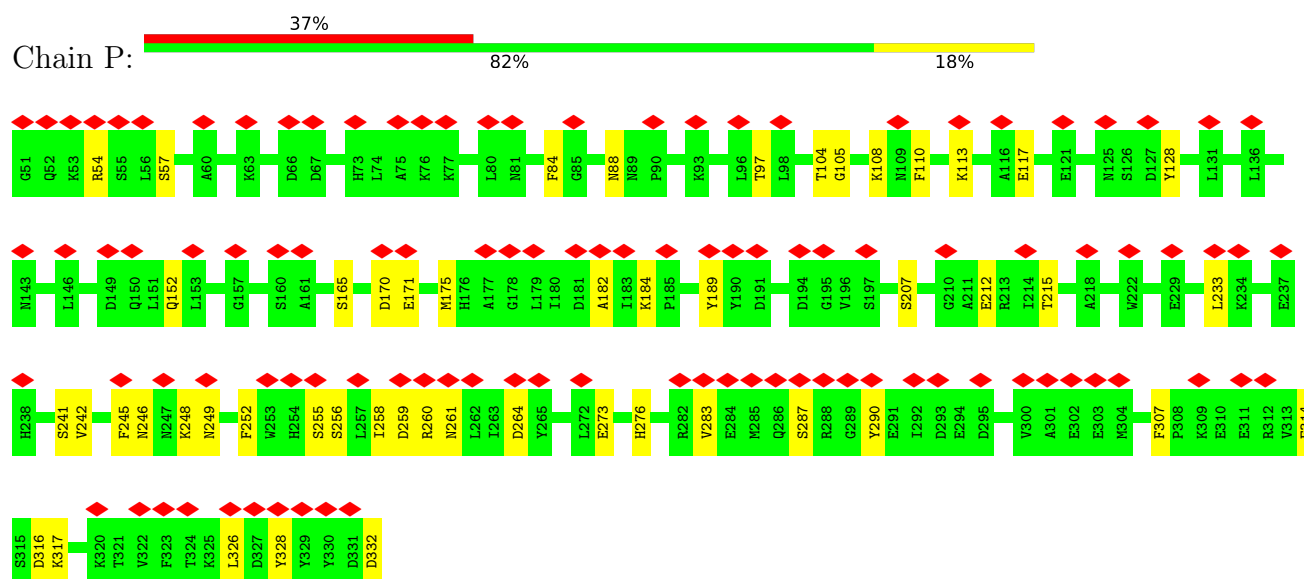
- Molecule 1: Torsin-1A



- Molecule 1: Torsin-1A



- Molecule 1: Torsin-1A



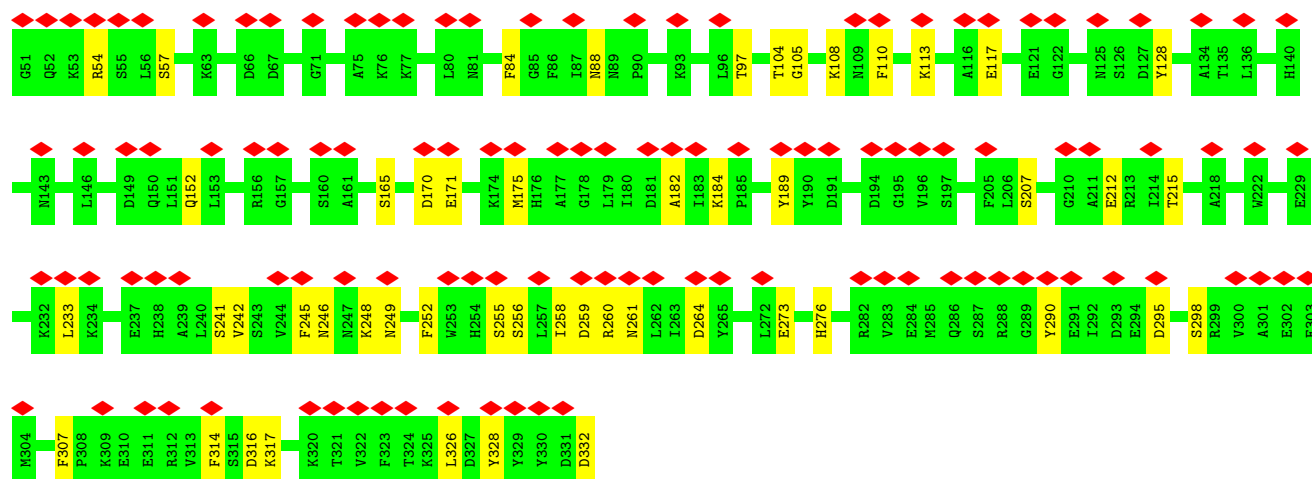
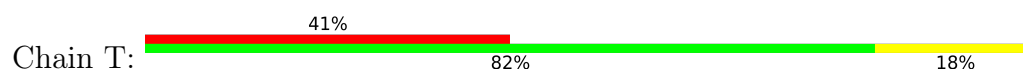
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	Y189	S57
L272	Y190	Q62
E273	D191	
	L192	L65
H276		D66
Q286	G195	D67
S287	Q199	
R288		F84
Q289	F205	G85
E291	L206	
L292	S207	N88
D293		P92
E294	E112	
D295	T215	T97
	D216	
S298	L219	G102
R299	D220	I103
V300		T104
A301	R223	G105
E302	S224	
E303	G225	H108
M304	K226	F110
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F307	R228	
F308		Y128
K309	L233	V129
E310	K234	H130
E311		A134
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S315	L240	A141
D316	S241	
K317	V242	Q152
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	F245	D170
T321	N246	E171
F322	N247	
T324	K248	M172
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L326	S250	K174
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D327	F252	H176
Y328		A177
Y329	H254	G178
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D332		
	L258	
	D259	
	S260	

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K234	E237	H238	A239	L240	S241	V242	F245	N246	H247	K248	N249	F252	W253	H254	S255	S256	L257	L258	D259	R260	N261	L262	L263	D264	Y265	L272	E273	H276	R282	V283	E284	M285	Q286	S287	R288	C289	Y290	E291	I292	D295	S296	R299	V300	A301	E302	E303	M304	F307	F308	K309
G51	Q52	K53	R54	S55	L56	S57	K63	D66	D67	G71	Q72	H73	L74	A75	K76	K77	L80	N81	F84	N88	N89	P90	K93	L96	T97	L98	T104	G105	K108	N109	F110	K113	A116	E117	E121	L124	N125	S126	D127	Y128	L136	H140	A141							
S142	N143	L146	D149	Q150	L151	Q152	L153	R156	G157	S160	A161	S165	D170	E171	K174	M175	H176	A177	G178	L179	T180	D181	A182	I183	K184	P185	Y189	V190	D191	D194	G195	V196	S197	L206	S207	G210	A211	E212	R213	T214	T215	A218	E229	K232	L233					

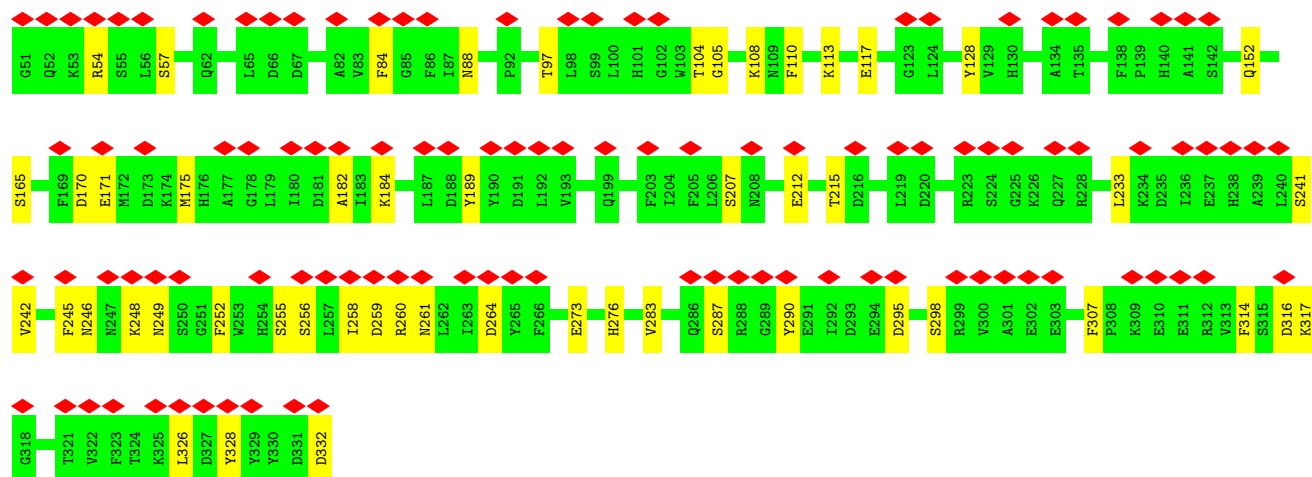
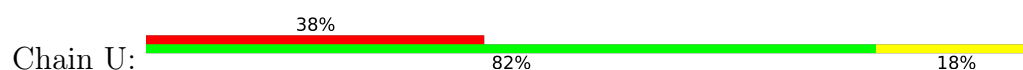
N246	N247	N248	N249	N250	N251	N252	N253	N254	N255	N256	N257	N258	N259	N260	N261	N262	N263	N264	N265	N266	N267	N268	N269	N270	N271	N272	N273	N274	N275	N276	N277	N278	N279	N280	N281	N282	N283	N284	N285	N286	N287	N288	N289	N290	N291	N292	N293	N294	N295	N296	N297	N298	N299	N300	N301	N302	N303	N304	N305	N306	N307	N308	N309	N310	N311	N312	N313	N314	N315	N316	N317	N318	N319	N320	N321	N322	N323	N324	N325	N326	N327	N328	N329	N330	N331	N332	N333	N334	N335	N336	N337	N338	N339	N340	N341	N342	N343	N344	N345	N346	N347	N348	N349	N350	N351	N352	N353	N354	N355	N356	N357	N358	N359	N360	N361	N362	N363	N364	N365	N366	N367	N368	N369	N370	N371	N372	N373	N374	N375	N376	N377	N378	N379	N380	N381	N382	N383	N384	N385	N386	N387	N388	N389	N390	N391	N392	N393	N394	N395	N396	N397	N398	N399	N400	N401	N402	N403	N404	N405	N406	N407	N408	N409	N410	N411	N412	N413	N414	N415	N416	N417	N418	N419	N420	N421	N422	N423	N424	N425	N426	N427	N428	N429	N430	N431	N432	N433	N434	N435	N436	N437	N438	N439	N440	N441	N442	N443	N444	N445	N446	N447	N448	N449	N450	N451	N452	N453	N454	N455	N456	N457	N458	N459	N460	N461	N462	N463	N464	N465	N466	N467	N468	N469	N470	N471	N472	N473	N474	N475	N476	N477	N478	N479	N480	N481	N482	N483	N484	N485	N486	N487	N488	N489	N490	N491	N492	N493	N494	N495	N496	N497	N498	N499	N500	N501	N502	N503	N504	N505	N506	N507	N508	N509	N510	N511	N512	N513	N514	N515	N516	N517	N518	N519	N520	N521	N522	N523	N524	N525	N526	N527	N528	N529	N530	N531	N532	N533	N534	N535	N536	N537	N538	N539	N540	N541	N542	N543	N544	N545	N546	N547	N548	N549	N550	N551	N552	N553	N554	N555	N556	N557	N558	N559	N560	N561	N562	N563	N564	N565	N566	N567	N568	N569	N570	N571	N572	N573	N574	N575	N576	N577	N578	N579	N580	N581	N582	N583	N584	N585	N586	N587	N588	N589	N590	N591	N592	N593	N594	N595	N596	N597	N598	N599	N600	N601	N602	N603	N604	N605	N606	N607	N608	N609	N610	N611	N612	N613	N614	N615	N616	N617	N618	N619	N620	N621	N622	N623	N624	N625	N626	N627	N628	N629	N630	N631	N632	N633	N634	N635	N636	N637	N638	N639	N640	N641	N642	N643	N644	N645	N646	N647	N648	N649	N650	N651	N652	N653	N654	N655	N656	N657	N658	N659	N660	N661	N662	N663	N664	N665	N666	N667	N668	N669	N670	N671	N672	N673	N674	N675	N676	N677	N678	N679	N680	N681	N682	N683	N684	N685	N686	N687	N688	N689	N690	N691	N692	N693	N694	N695	N696	N697	N698	N699	N700	N701	N702	N703	N704	N705	N706	N707	N708	N709	N710	N711	N712	N713	N714	N715	N716	N717	N718	N719	N720	N721	N722	N723	N724	N725	N726	N727	N728	N729	N730	N731	N732	N733	N734	N735	N736	N737	N738	N739	N740	N741	N742	N743	N744	N745	N746	N747	N748	N749	N750	N751	N752	N753	N754	N755	N756
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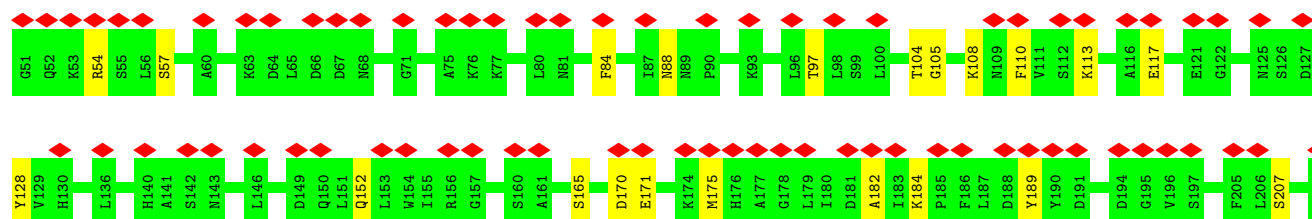
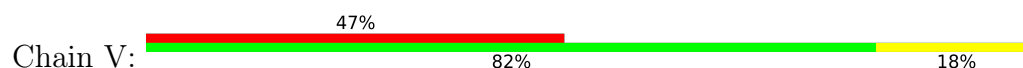
• Molecule 1: Torsin-1A

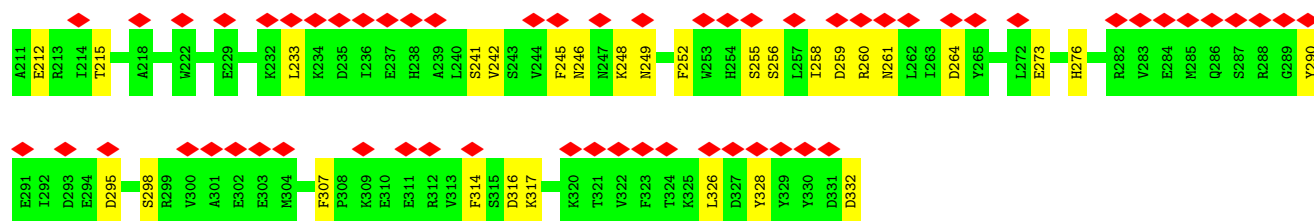


• Molecule 1: Torsin-1A

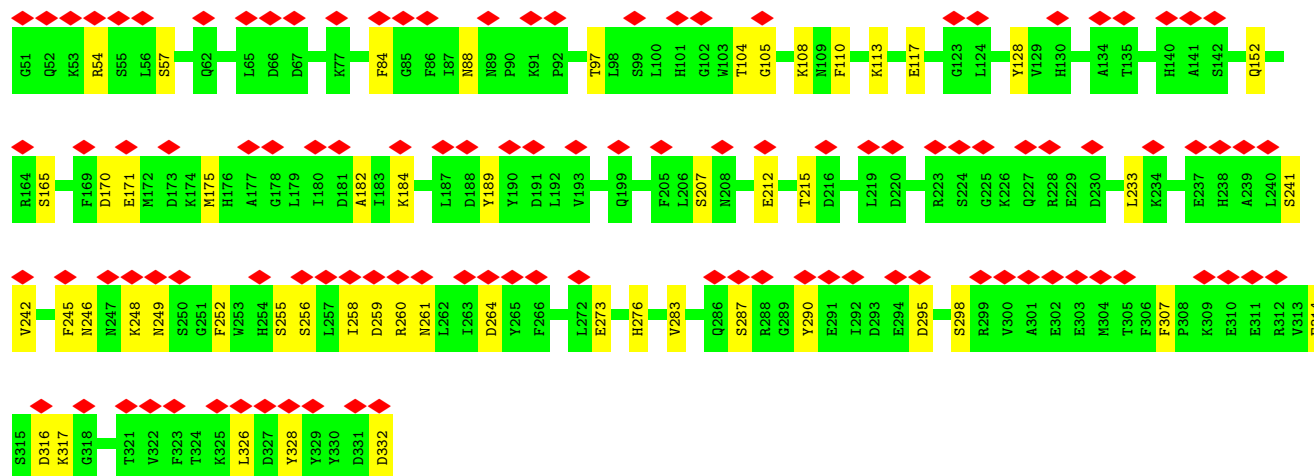
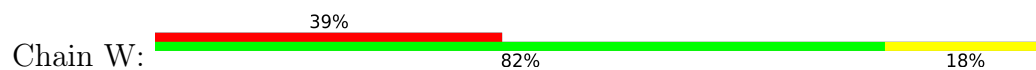


• Molecule 1: Torsin-1A

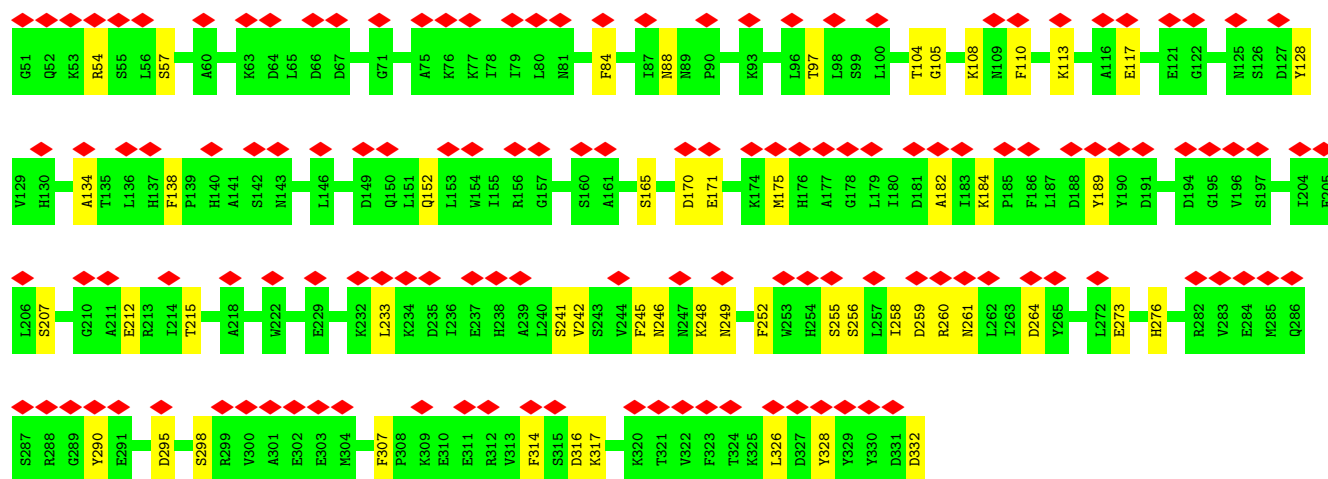
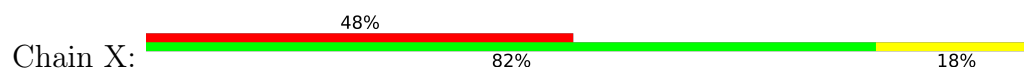




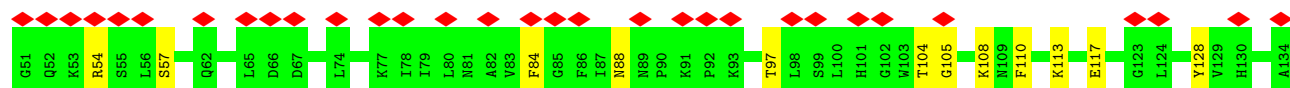
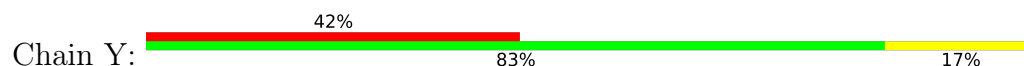
• Molecule 1: Torsin-1A

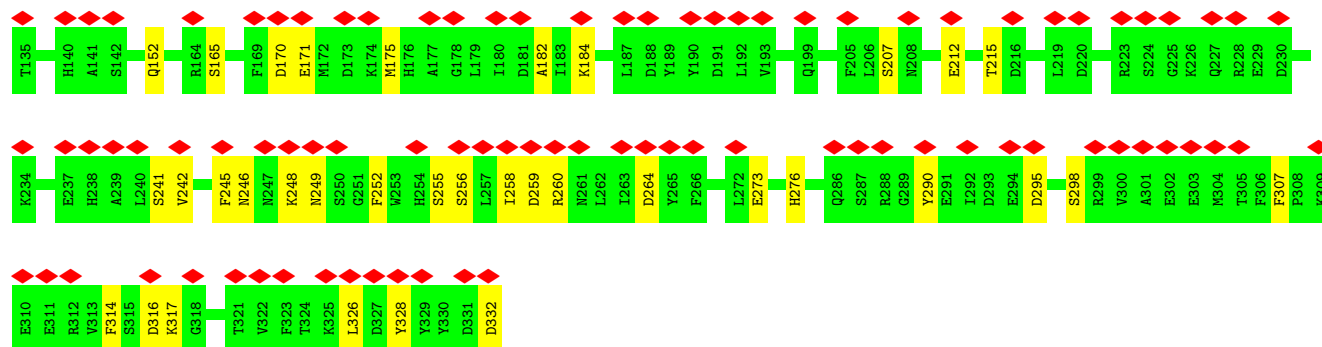


• Molecule 1: Torsin-1A



• Molecule 1: Torsin-1A





4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=42.51°, rise=5.53 Å, axial sym=C1	Depositor
Number of segments used	75909	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{Å}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.722	Depositor
Minimum map value	-0.246	Depositor
Average map value	0.028	Depositor
Map value standard deviation	0.092	Depositor
Recommended contour level	0.247	Depositor
Map size (Å)	224.448, 224.448, 224.448	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.169, 1.169, 1.169	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	0.35	0/2356	0.58	0/3177
1	B	0.35	0/2356	0.59	0/3177
1	C	0.35	0/2356	0.59	0/3177
1	D	0.35	0/2356	0.59	0/3177
1	E	0.35	0/2356	0.58	0/3177
1	F	0.35	0/2356	0.59	0/3177
1	G	0.35	0/2356	0.58	0/3177
1	H	0.35	0/2356	0.58	0/3177
1	I	0.35	0/2356	0.59	0/3177
1	J	0.35	0/2356	0.59	0/3177
1	K	0.35	0/2356	0.59	0/3177
1	L	0.35	0/2356	0.59	0/3177
1	M	0.35	0/2356	0.59	0/3177
1	N	0.35	0/2356	0.59	0/3177
1	O	0.35	0/2356	0.59	0/3177
1	P	0.35	0/2356	0.59	0/3177
1	Q	0.35	0/2356	0.58	0/3177
1	R	0.35	0/2356	0.58	0/3177
1	S	0.35	0/2356	0.58	0/3177
1	T	0.35	0/2356	0.59	0/3177
1	U	0.35	0/2356	0.59	0/3177
1	V	0.35	0/2356	0.58	0/3177
1	W	0.35	0/2356	0.59	0/3177
1	X	0.35	0/2356	0.59	0/3177
1	Y	0.35	0/2356	0.58	0/3177
All	All	0.35	0/58900	0.59	0/79425

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2300	2270	2266	31	0
1	B	2300	2270	2266	31	0
1	C	2300	2270	2266	29	0
1	D	2300	2270	2266	32	0
1	E	2300	2270	2266	33	0
1	F	2300	2270	2266	31	0
1	G	2300	2270	2266	31	0
1	H	2300	2270	2266	32	0
1	I	2300	2270	2266	31	0
1	J	2300	2270	2266	31	0
1	K	2300	2270	2266	31	0
1	L	2300	2270	2266	30	0
1	M	2300	2270	2266	31	0
1	N	2300	2270	2266	32	0
1	O	2300	2270	2266	31	0
1	P	2300	2270	2266	32	0
1	Q	2300	2270	2266	31	0
1	R	2300	2270	2266	32	0
1	S	2300	2270	2266	31	0
1	T	2300	2270	2266	31	0
1	U	2300	2270	2266	32	0
1	V	2300	2270	2266	31	0
1	W	2300	2270	2266	33	0
1	X	2300	2270	2266	30	0
1	Y	2300	2270	2267	26	0
2	A	31	12	12	4	0
2	B	31	12	12	5	0
2	C	31	12	12	5	0
2	D	31	12	12	4	0
2	E	31	12	12	4	0
2	F	31	12	12	4	0
2	G	31	12	12	4	0
2	H	31	12	12	4	0
2	I	31	12	12	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	31	12	12	4	0
2	K	31	12	12	4	0
2	L	31	12	12	4	0
2	M	31	12	12	4	0
2	N	31	12	12	4	0
2	O	31	12	12	5	0
2	P	31	12	12	5	0
2	Q	31	12	12	5	0
2	R	31	12	12	5	0
2	S	31	12	12	4	0
2	T	31	12	12	5	0
2	U	31	12	12	5	0
2	V	31	12	12	4	0
2	W	31	12	12	4	0
2	X	62	24	24	5	0
All	All	58275	57050	56951	728	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (728) 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:C:189:TYR:CE1	2:C:401:ATP:O2A	1.91	1.10
1:I:189:TYR:CE1	2:I:401:ATP:O2A	1.91	1.09
1:T:189:TYR:CE1	2:T:401:ATP:O2A	1.91	1.08
1:F:189:TYR:CE1	2:F:401:ATP:O2A	1.91	1.07
1:L:189:TYR:CE1	2:L:401:ATP:O2A	1.91	1.06
1:S:189:TYR:CE1	2:S:401:ATP:O2A	1.91	1.05
1:D:189:TYR:CE1	2:D:401:ATP:O2A	1.91	1.05
1:R:189:TYR:CE1	2:R:401:ATP:O2A	1.91	1.05
1:H:189:TYR:CE1	2:H:401:ATP:O2A	1.91	1.05
1:M:189:TYR:CE1	2:M:401:ATP:O2A	1.91	1.03
1:U:189:TYR:CE1	2:U:401:ATP:O2A	1.91	1.02
1:K:189:TYR:CE1	2:K:401:ATP:O2A	1.91	1.02
1:G:189:TYR:CE1	2:G:401:ATP:O2A	1.91	1.02
1:E:189:TYR:CE1	2:E:401:ATP:O2A	1.91	1.01
1:N:189:TYR:CE1	2:N:401:ATP:O2A	1.91	1.00
1:J:189:TYR:CE1	2:J:401:ATP:O2A	1.91	1.00
1:B:189:TYR:CE1	2:B:401:ATP:O2A	1.91	0.99
1:P:189:TYR:CE1	2:P:401:ATP:O2A	1.91	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:189:TYR:CE1	2:W:401:ATP:O2A	1.91	0.98
1:O:189:TYR:CE1	2:O:401:ATP:O2A	1.91	0.98
1:Q:189:TYR:CE1	2:Q:401:ATP:O2A	1.91	0.97
1:A:189:TYR:CE1	2:A:401:ATP:O2A	1.91	0.97
1:V:189:TYR:CE1	2:V:401:ATP:O2A	1.91	0.96
1:X:189:TYR:CE1	2:X:401:ATP:O2A	1.91	0.96
1:W:189:TYR:HE1	2:W:401:ATP:O2A	1.48	0.93
1:U:189:TYR:HE1	2:U:401:ATP:O2A	1.48	0.91
1:O:189:TYR:HE1	2:O:401:ATP:O2A	1.48	0.91
1:G:189:TYR:HE1	2:G:401:ATP:O2A	1.48	0.91
1:E:189:TYR:HE1	2:E:401:ATP:O2A	1.48	0.90
1:T:189:TYR:HE1	2:T:401:ATP:O2A	1.48	0.90
1:V:189:TYR:HE1	2:V:401:ATP:O2A	1.48	0.90
1:I:189:TYR:HE1	2:I:401:ATP:O2A	1.48	0.89
1:L:189:TYR:HE1	2:L:401:ATP:O2A	1.48	0.88
1:S:189:TYR:HE1	2:S:401:ATP:O2A	1.48	0.88
1:C:189:TYR:HE1	2:C:401:ATP:O2A	1.48	0.88
1:R:189:TYR:HE1	2:R:401:ATP:O2A	1.48	0.88
1:J:189:TYR:HE1	2:J:401:ATP:O2A	1.48	0.88
1:X:189:TYR:HE1	2:X:401:ATP:O2A	1.48	0.88
1:N:189:TYR:HE1	2:N:401:ATP:O2A	1.48	0.88
1:D:189:TYR:HE1	2:D:401:ATP:O2A	1.48	0.87
1:B:189:TYR:HE1	2:B:401:ATP:O2A	1.48	0.87
1:F:189:TYR:HE1	2:F:401:ATP:O2A	1.48	0.87
1:H:189:TYR:HE1	2:H:401:ATP:O2A	1.48	0.86
1:K:189:TYR:HE1	2:K:401:ATP:O2A	1.48	0.86
1:P:189:TYR:HE1	2:P:401:ATP:O2A	1.48	0.85
1:A:189:TYR:HE1	2:A:401:ATP:O2A	1.48	0.85
1:M:189:TYR:HE1	2:M:401:ATP:O2A	1.48	0.85
1:Q:189:TYR:HE1	2:Q:401:ATP:O2A	1.48	0.85
1:C:290:TYR:OH	1:C:326:LEU:O	2.04	0.76
1:W:290:TYR:OH	1:W:326:LEU:O	2.04	0.76
1:L:290:TYR:OH	1:L:326:LEU:O	2.04	0.76
1:S:290:TYR:OH	1:S:326:LEU:O	2.04	0.76
1:R:290:TYR:OH	1:R:326:LEU:O	2.04	0.76
1:M:108:LYS:NZ	1:M:207:SER:O	2.19	0.76
1:C:108:LYS:NZ	1:C:207:SER:O	2.19	0.76
1:A:108:LYS:NZ	1:A:207:SER:O	2.19	0.76
1:J:108:LYS:NZ	1:J:207:SER:O	2.19	0.76
1:P:108:LYS:NZ	1:P:207:SER:O	2.19	0.76
1:Q:290:TYR:OH	1:Q:326:LEU:O	2.04	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:108:LYS:NZ	1:S:207:SER:O	2.19	0.76
1:D:108:LYS:NZ	1:D:207:SER:O	2.19	0.76
1:N:108:LYS:NZ	1:N:207:SER:O	2.19	0.76
1:N:290:TYR:OH	1:N:326:LEU:O	2.04	0.76
1:P:290:TYR:OH	1:P:326:LEU:O	2.04	0.76
1:X:108:LYS:NZ	1:X:207:SER:O	2.19	0.76
1:B:290:TYR:OH	1:B:326:LEU:O	2.04	0.76
1:G:290:TYR:OH	1:G:326:LEU:O	2.04	0.76
1:I:290:TYR:OH	1:I:326:LEU:O	2.04	0.76
1:R:108:LYS:NZ	1:R:207:SER:O	2.19	0.76
1:U:108:LYS:NZ	1:U:207:SER:O	2.19	0.76
1:E:290:TYR:OH	1:E:326:LEU:O	2.04	0.76
1:F:108:LYS:NZ	1:F:207:SER:O	2.19	0.76
1:E:108:LYS:NZ	1:E:207:SER:O	2.19	0.76
1:G:108:LYS:NZ	1:G:207:SER:O	2.19	0.76
1:Q:108:LYS:NZ	1:Q:207:SER:O	2.19	0.76
1:V:108:LYS:NZ	1:V:207:SER:O	2.19	0.76
1:H:108:LYS:NZ	1:H:207:SER:O	2.19	0.75
1:K:108:LYS:NZ	1:K:207:SER:O	2.19	0.75
1:Y:290:TYR:OH	1:Y:326:LEU:O	2.04	0.75
1:B:108:LYS:NZ	1:B:207:SER:O	2.19	0.75
1:D:290:TYR:OH	1:D:326:LEU:O	2.04	0.75
1:T:108:LYS:NZ	1:T:207:SER:O	2.19	0.75
1:I:108:LYS:NZ	1:I:207:SER:O	2.19	0.75
1:O:108:LYS:NZ	1:O:207:SER:O	2.18	0.75
1:L:108:LYS:NZ	1:L:207:SER:O	2.19	0.75
1:U:290:TYR:OH	1:U:326:LEU:O	2.04	0.75
1:W:108:LYS:NZ	1:W:207:SER:O	2.19	0.75
1:Y:108:LYS:NZ	1:Y:207:SER:O	2.19	0.75
1:A:290:TYR:OH	1:A:326:LEU:O	2.04	0.75
1:K:290:TYR:OH	1:K:326:LEU:O	2.04	0.75
1:T:290:TYR:OH	1:T:326:LEU:O	2.04	0.75
1:F:290:TYR:OH	1:F:326:LEU:O	2.04	0.75
1:H:290:TYR:OH	1:H:326:LEU:O	2.04	0.75
1:J:290:TYR:OH	1:J:326:LEU:O	2.04	0.75
1:M:290:TYR:OH	1:M:326:LEU:O	2.04	0.74
1:X:290:TYR:OH	1:X:326:LEU:O	2.04	0.74
1:O:290:TYR:OH	1:O:326:LEU:O	2.04	0.74
1:V:290:TYR:OH	1:V:326:LEU:O	2.04	0.73
1:V:259:ASP:O	1:V:260:ARG:NE	2.28	0.67
1:K:259:ASP:O	1:K:260:ARG:NE	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:259:ASP:O	1:I:260:ARG:NE	2.28	0.67
1:T:259:ASP:O	1:T:260:ARG:NE	2.28	0.67
1:C:259:ASP:O	1:C:260:ARG:NE	2.28	0.67
1:M:259:ASP:O	1:M:260:ARG:NE	2.28	0.67
1:R:259:ASP:O	1:R:260:ARG:NE	2.28	0.67
1:U:259:ASP:O	1:U:260:ARG:NE	2.28	0.67
1:L:259:ASP:O	1:L:260:ARG:NE	2.28	0.66
1:J:259:ASP:O	1:J:260:ARG:NE	2.28	0.66
1:O:259:ASP:O	1:O:260:ARG:NE	2.28	0.66
1:W:259:ASP:O	1:W:260:ARG:NE	2.28	0.66
1:P:259:ASP:O	1:P:260:ARG:NE	2.28	0.66
1:Q:259:ASP:O	1:Q:260:ARG:NE	2.28	0.66
1:H:259:ASP:O	1:H:260:ARG:NE	2.28	0.66
1:E:259:ASP:O	1:E:260:ARG:NE	2.28	0.65
1:Y:259:ASP:O	1:Y:260:ARG:NE	2.28	0.65
1:A:54:ARG:NH2	1:A:57:SER:OG	2.30	0.65
1:E:328:TYR:O	1:E:332:ASP:N	2.30	0.65
1:L:54:ARG:NH2	1:L:57:SER:OG	2.30	0.65
1:M:54:ARG:NH2	1:M:57:SER:OG	2.30	0.65
1:T:54:ARG:NH2	1:T:57:SER:OG	2.30	0.65
1:H:54:ARG:NH2	1:H:57:SER:OG	2.30	0.65
1:K:54:ARG:NH2	1:K:57:SER:OG	2.30	0.65
1:L:328:TYR:O	1:L:332:ASP:N	2.30	0.65
1:N:328:TYR:O	1:N:332:ASP:N	2.30	0.65
1:C:328:TYR:O	1:C:332:ASP:N	2.30	0.65
1:G:54:ARG:NH2	1:G:57:SER:OG	2.30	0.65
1:G:328:TYR:O	1:G:332:ASP:N	2.30	0.65
1:P:328:TYR:O	1:P:332:ASP:N	2.30	0.65
1:U:54:ARG:NH2	1:U:57:SER:OG	2.30	0.65
1:W:54:ARG:NH2	1:W:57:SER:OG	2.30	0.65
1:W:328:TYR:O	1:W:332:ASP:N	2.30	0.65
1:O:54:ARG:NH2	1:O:57:SER:OG	2.30	0.65
1:U:328:TYR:O	1:U:332:ASP:N	2.30	0.65
1:C:54:ARG:NH2	1:C:57:SER:OG	2.30	0.65
1:S:54:ARG:NH2	1:S:57:SER:OG	2.30	0.65
1:Y:328:TYR:O	1:Y:332:ASP:N	2.30	0.65
1:B:54:ARG:NH2	1:B:57:SER:OG	2.30	0.65
1:F:54:ARG:NH2	1:F:57:SER:OG	2.30	0.65
1:J:328:TYR:O	1:J:332:ASP:N	2.30	0.65
1:V:54:ARG:NH2	1:V:57:SER:OG	2.30	0.65
1:X:54:ARG:NH2	1:X:57:SER:OG	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:54:ARG:NH2	1:Y:57:SER:OG	2.30	0.65
1:E:54:ARG:NH2	1:E:57:SER:OG	2.30	0.65
1:N:54:ARG:NH2	1:N:57:SER:OG	2.30	0.65
1:R:54:ARG:NH2	1:R:57:SER:OG	2.30	0.65
1:A:328:TYR:O	1:A:332:ASP:N	2.30	0.65
1:F:259:ASP:O	1:F:260:ARG:NE	2.28	0.65
1:I:328:TYR:O	1:I:332:ASP:N	2.30	0.65
1:S:259:ASP:O	1:S:260:ARG:NE	2.28	0.65
1:S:328:TYR:O	1:S:332:ASP:N	2.30	0.65
1:J:54:ARG:NH2	1:J:57:SER:OG	2.30	0.64
1:U:128:TYR:O	1:U:165:SER:OG	2.15	0.64
1:R:328:TYR:O	1:R:332:ASP:N	2.30	0.64
1:Y:128:TYR:O	1:Y:165:SER:OG	2.15	0.64
1:I:54:ARG:NH2	1:I:57:SER:OG	2.30	0.64
1:W:128:TYR:O	1:W:165:SER:OG	2.15	0.64
1:D:54:ARG:NH2	1:D:57:SER:OG	2.30	0.64
1:K:316:ASP:OD2	1:K:317:LYS:NZ	2.31	0.64
1:S:128:TYR:O	1:S:165:SER:OG	2.15	0.64
1:V:328:TYR:O	1:V:332:ASP:N	2.30	0.64
1:M:316:ASP:OD2	1:M:317:LYS:NZ	2.31	0.64
1:P:54:ARG:NH2	1:P:57:SER:OG	2.30	0.64
1:E:128:TYR:O	1:E:165:SER:OG	2.15	0.64
1:F:316:ASP:OD2	1:F:317:LYS:NZ	2.31	0.64
1:G:128:TYR:O	1:G:165:SER:OG	2.15	0.64
1:H:316:ASP:OD2	1:H:317:LYS:NZ	2.31	0.64
1:J:316:ASP:OD2	1:J:317:LYS:NZ	2.31	0.64
1:N:259:ASP:O	1:N:260:ARG:NE	2.28	0.64
1:Q:54:ARG:NH2	1:Q:57:SER:OG	2.30	0.64
1:C:128:TYR:O	1:C:165:SER:OG	2.15	0.64
1:H:328:TYR:O	1:H:332:ASP:N	2.30	0.64
1:I:128:TYR:O	1:I:165:SER:OG	2.15	0.64
1:I:316:ASP:OD2	1:I:317:LYS:NZ	2.31	0.64
1:T:328:TYR:O	1:T:332:ASP:N	2.30	0.64
1:X:316:ASP:OD2	1:X:317:LYS:NZ	2.31	0.64
1:D:316:ASP:OD2	1:D:317:LYS:NZ	2.31	0.64
1:D:328:TYR:O	1:D:332:ASP:N	2.30	0.64
1:T:316:ASP:OD2	1:T:317:LYS:NZ	2.31	0.64
1:X:328:TYR:O	1:X:332:ASP:N	2.30	0.64
1:D:259:ASP:O	1:D:260:ARG:NE	2.28	0.64
1:F:328:TYR:O	1:F:332:ASP:N	2.30	0.64
1:O:316:ASP:OD2	1:O:317:LYS:NZ	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:328:TYR:O	1:Q:332:ASP:N	2.30	0.64
1:V:316:ASP:OD2	1:V:317:LYS:NZ	2.31	0.64
1:Y:316:ASP:OD2	1:Y:317:LYS:NZ	2.31	0.64
1:K:328:TYR:O	1:K:332:ASP:N	2.30	0.63
1:P:316:ASP:OD2	1:P:317:LYS:NZ	2.31	0.63
1:S:316:ASP:OD2	1:S:317:LYS:NZ	2.31	0.63
1:B:328:TYR:O	1:B:332:ASP:N	2.30	0.63
1:C:316:ASP:OD2	1:C:317:LYS:NZ	2.31	0.63
1:G:259:ASP:O	1:G:260:ARG:NE	2.28	0.63
1:Q:128:TYR:O	1:Q:165:SER:OG	2.15	0.63
1:N:128:TYR:O	1:N:165:SER:OG	2.15	0.63
1:B:316:ASP:OD2	1:B:317:LYS:NZ	2.31	0.63
1:J:128:TYR:O	1:J:165:SER:OG	2.15	0.63
1:L:128:TYR:O	1:L:165:SER:OG	2.15	0.63
1:M:328:TYR:O	1:M:332:ASP:N	2.30	0.63
1:H:128:TYR:O	1:H:165:SER:OG	2.15	0.63
1:M:128:TYR:O	1:M:165:SER:OG	2.15	0.63
1:G:316:ASP:OD2	1:G:317:LYS:NZ	2.31	0.63
1:L:316:ASP:OD2	1:L:317:LYS:NZ	2.31	0.63
1:O:328:TYR:O	1:O:332:ASP:N	2.30	0.63
1:Q:316:ASP:OD2	1:Q:317:LYS:NZ	2.31	0.63
1:J:248:LYS:O	1:J:252:PHE:N	2.32	0.63
1:K:248:LYS:O	1:K:252:PHE:N	2.32	0.63
1:O:128:TYR:O	1:O:165:SER:OG	2.15	0.63
1:P:128:TYR:O	1:P:165:SER:OG	2.15	0.63
1:R:316:ASP:OD2	1:R:317:LYS:NZ	2.31	0.63
1:W:248:LYS:O	1:W:252:PHE:N	2.32	0.63
1:W:316:ASP:OD2	1:W:317:LYS:NZ	2.31	0.63
1:Y:248:LYS:O	1:Y:252:PHE:N	2.32	0.63
1:B:259:ASP:O	1:B:260:ARG:NE	2.28	0.63
1:E:248:LYS:O	1:E:252:PHE:N	2.32	0.63
1:F:128:TYR:O	1:F:165:SER:OG	2.15	0.63
1:X:241:SER:O	1:X:245:PHE:N	2.32	0.63
1:A:316:ASP:OD2	1:A:317:LYS:NZ	2.31	0.62
1:H:248:LYS:O	1:H:252:PHE:N	2.32	0.62
1:U:316:ASP:OD2	1:U:317:LYS:NZ	2.31	0.62
1:E:316:ASP:OD2	1:E:317:LYS:NZ	2.31	0.62
1:F:241:SER:O	1:F:245:PHE:N	2.32	0.62
1:X:248:LYS:O	1:X:252:PHE:N	2.32	0.62
1:H:241:SER:O	1:H:245:PHE:N	2.32	0.62
1:I:248:LYS:O	1:I:252:PHE:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:241:SER:O	1:P:245:PHE:N	2.32	0.62
1:R:128:TYR:O	1:R:165:SER:OG	2.15	0.62
1:T:128:TYR:O	1:T:165:SER:OG	2.15	0.62
1:X:128:TYR:O	1:X:165:SER:OG	2.15	0.62
1:L:248:LYS:O	1:L:252:PHE:N	2.32	0.62
1:N:316:ASP:OD2	1:N:317:LYS:NZ	2.31	0.62
1:C:241:SER:O	1:C:245:PHE:N	2.32	0.62
1:G:248:LYS:O	1:G:252:PHE:N	2.32	0.62
1:K:241:SER:O	1:K:245:PHE:N	2.32	0.62
1:B:128:TYR:O	1:B:165:SER:OG	2.16	0.62
1:O:241:SER:O	1:O:245:PHE:N	2.32	0.62
1:U:248:LYS:O	1:U:252:PHE:N	2.32	0.62
1:V:128:TYR:O	1:V:165:SER:OG	2.15	0.62
1:U:241:SER:O	1:U:245:PHE:N	2.32	0.61
1:A:241:SER:O	1:A:245:PHE:N	2.32	0.61
1:A:259:ASP:O	1:A:260:ARG:NE	2.28	0.61
1:D:128:TYR:O	1:D:165:SER:OG	2.15	0.61
1:S:241:SER:O	1:S:245:PHE:N	2.32	0.61
1:I:241:SER:O	1:I:245:PHE:N	2.32	0.61
1:J:241:SER:O	1:J:245:PHE:N	2.32	0.61
1:N:241:SER:O	1:N:245:PHE:N	2.32	0.61
1:B:241:SER:O	1:B:245:PHE:N	2.32	0.61
1:D:248:LYS:O	1:D:252:PHE:N	2.32	0.61
1:Q:241:SER:O	1:Q:245:PHE:N	2.32	0.61
1:R:241:SER:O	1:R:245:PHE:N	2.32	0.61
1:D:241:SER:O	1:D:245:PHE:N	2.32	0.61
1:A:128:TYR:O	1:A:165:SER:OG	2.15	0.61
1:T:241:SER:O	1:T:245:PHE:N	2.32	0.61
1:X:259:ASP:O	1:X:260:ARG:NE	2.28	0.61
1:F:248:LYS:O	1:F:252:PHE:N	2.32	0.61
1:E:241:SER:O	1:E:245:PHE:N	2.32	0.61
1:N:248:LYS:O	1:N:252:PHE:N	2.32	0.61
1:A:248:LYS:O	1:A:252:PHE:N	2.32	0.60
1:R:248:LYS:O	1:R:252:PHE:N	2.32	0.60
1:V:241:SER:O	1:V:245:PHE:N	2.32	0.60
1:O:248:LYS:O	1:O:252:PHE:N	2.32	0.60
1:S:248:LYS:O	1:S:252:PHE:N	2.32	0.60
1:G:241:SER:O	1:G:245:PHE:N	2.32	0.60
1:L:241:SER:O	1:L:245:PHE:N	2.32	0.60
1:M:241:SER:O	1:M:245:PHE:N	2.32	0.60
1:P:248:LYS:O	1:P:252:PHE:N	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:241:SER:O	1:Y:245:PHE:N	2.32	0.60
1:Q:248:LYS:O	1:Q:252:PHE:N	2.32	0.60
1:T:248:LYS:O	1:T:252:PHE:N	2.32	0.60
1:W:241:SER:O	1:W:245:PHE:N	2.32	0.60
1:B:248:LYS:O	1:B:252:PHE:N	2.32	0.59
1:K:128:TYR:O	1:K:165:SER:OG	2.15	0.59
1:V:248:LYS:O	1:V:252:PHE:N	2.32	0.59
1:L:307:PHE:N	1:L:314:PHE:O	2.36	0.59
1:C:248:LYS:O	1:C:252:PHE:N	2.32	0.59
1:G:307:PHE:N	1:G:314:PHE:O	2.36	0.59
1:M:248:LYS:O	1:M:252:PHE:N	2.32	0.59
1:W:307:PHE:N	1:W:314:PHE:O	2.36	0.59
1:H:307:PHE:N	1:H:314:PHE:O	2.36	0.59
1:I:273:GLU:O	1:I:276:HIS:N	2.37	0.58
1:L:273:GLU:O	1:L:276:HIS:N	2.37	0.58
1:O:273:GLU:O	1:O:276:HIS:N	2.37	0.58
1:Q:273:GLU:O	1:Q:276:HIS:N	2.37	0.58
1:D:273:GLU:O	1:D:276:HIS:N	2.37	0.58
1:G:273:GLU:O	1:G:276:HIS:N	2.37	0.58
1:N:273:GLU:O	1:N:276:HIS:N	2.37	0.58
1:R:273:GLU:O	1:R:276:HIS:N	2.37	0.58
1:F:273:GLU:O	1:F:276:HIS:N	2.37	0.58
1:I:307:PHE:N	1:I:314:PHE:O	2.36	0.58
1:P:273:GLU:O	1:P:276:HIS:N	2.37	0.58
1:S:273:GLU:O	1:S:276:HIS:N	2.37	0.58
1:F:189:TYR:CE1	2:F:401:ATP:H5'2	2.39	0.58
1:U:273:GLU:O	1:U:276:HIS:N	2.37	0.58
1:X:273:GLU:O	1:X:276:HIS:N	2.37	0.58
1:J:189:TYR:CE1	2:J:401:ATP:H5'2	2.39	0.58
1:M:307:PHE:N	1:M:314:PHE:O	2.36	0.58
1:R:189:TYR:CE1	2:R:401:ATP:H5'2	2.39	0.58
1:T:273:GLU:O	1:T:276:HIS:N	2.37	0.58
1:W:273:GLU:O	1:W:276:HIS:N	2.37	0.58
1:B:273:GLU:O	1:B:276:HIS:N	2.37	0.57
1:E:273:GLU:O	1:E:276:HIS:N	2.37	0.57
1:G:189:TYR:CE1	2:G:401:ATP:H5'2	2.39	0.57
1:J:273:GLU:O	1:J:276:HIS:N	2.37	0.57
1:K:189:TYR:CE1	2:K:401:ATP:H5'2	2.39	0.57
1:U:189:TYR:CE1	2:U:401:ATP:H5'2	2.39	0.57
1:V:189:TYR:CE1	2:V:401:ATP:H5'2	2.39	0.57
1:Q:189:TYR:CE1	2:Q:401:ATP:H5'2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:TYR:CE1	2:A:401:ATP:H5'2	2.39	0.57
1:E:189:TYR:CE1	2:E:401:ATP:H5'2	2.39	0.57
1:K:273:GLU:O	1:K:276:HIS:N	2.37	0.57
1:N:189:TYR:CE1	2:N:401:ATP:H5'2	2.39	0.57
1:O:189:TYR:CE1	2:O:401:ATP:H5'2	2.39	0.57
1:B:189:TYR:CE1	2:B:401:ATP:H5'2	2.39	0.57
1:T:189:TYR:CE1	2:T:401:ATP:H5'2	2.39	0.57
1:I:189:TYR:CE1	2:I:401:ATP:H5'2	2.39	0.57
1:M:189:TYR:CE1	2:M:401:ATP:H5'2	2.39	0.57
1:P:189:TYR:CE1	2:P:401:ATP:H5'2	2.39	0.57
1:V:273:GLU:O	1:V:276:HIS:N	2.37	0.57
1:A:110:PHE:N	2:B:401:ATP:O1A	2.34	0.57
2:A:401:ATP:O1A	1:C:110:PHE:N	2.34	0.57
1:J:307:PHE:N	1:J:314:PHE:O	2.36	0.57
1:X:189:TYR:CE1	2:X:401:ATP:H5'2	2.39	0.57
1:C:273:GLU:O	1:C:276:HIS:N	2.37	0.57
1:S:189:TYR:CE1	2:S:401:ATP:H5'2	2.39	0.57
1:T:110:PHE:N	2:V:401:ATP:O1A	2.34	0.57
1:W:189:TYR:CE1	2:W:401:ATP:H5'2	2.39	0.57
1:A:273:GLU:O	1:A:276:HIS:N	2.37	0.57
1:Y:273:GLU:O	1:Y:276:HIS:N	2.37	0.57
1:H:189:TYR:CE1	2:H:401:ATP:H5'2	2.39	0.57
1:L:189:TYR:CE1	2:L:401:ATP:H5'2	2.39	0.57
2:M:401:ATP:O1A	1:O:110:PHE:N	2.34	0.57
1:P:110:PHE:N	2:R:401:ATP:O1A	2.34	0.57
1:C:189:TYR:CE1	2:C:401:ATP:H5'2	2.39	0.56
1:D:189:TYR:CE1	2:D:401:ATP:H5'2	2.39	0.56
1:F:307:PHE:N	1:F:314:PHE:O	2.36	0.56
1:Y:307:PHE:N	1:Y:314:PHE:O	2.36	0.56
1:R:307:PHE:N	1:R:314:PHE:O	2.36	0.56
1:A:307:PHE:N	1:A:314:PHE:O	2.36	0.56
1:B:110:PHE:N	2:D:401:ATP:O1A	2.34	0.56
1:H:273:GLU:O	1:H:276:HIS:N	2.37	0.56
1:P:307:PHE:N	1:P:314:PHE:O	2.36	0.56
1:Q:307:PHE:N	1:Q:314:PHE:O	2.36	0.56
1:D:110:PHE:N	2:F:401:ATP:O1A	2.34	0.56
1:M:273:GLU:O	1:M:276:HIS:N	2.37	0.56
1:O:307:PHE:N	1:O:314:PHE:O	2.36	0.56
1:B:307:PHE:N	1:B:314:PHE:O	2.36	0.56
1:R:110:PHE:N	2:T:401:ATP:O1A	2.34	0.56
1:S:307:PHE:N	1:S:314:PHE:O	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:307:PHE:N	1:T:314:PHE:O	2.36	0.56
1:C:307:PHE:N	1:C:314:PHE:O	2.36	0.55
1:D:307:PHE:N	1:D:314:PHE:O	2.36	0.55
2:O:401:ATP:O1A	1:Q:110:PHE:N	2.34	0.55
1:N:307:PHE:N	1:N:314:PHE:O	2.36	0.55
2:C:401:ATP:O1A	1:E:110:PHE:N	2.34	0.54
1:V:307:PHE:N	1:V:314:PHE:O	2.36	0.54
1:U:307:PHE:N	1:U:314:PHE:O	2.36	0.54
1:X:307:PHE:N	1:X:314:PHE:O	2.36	0.54
1:V:110:PHE:N	2:X:401:ATP:O1A	2.34	0.54
1:C:175:MET:O	1:C:249:ASN:ND2	2.41	0.54
1:E:307:PHE:N	1:E:314:PHE:O	2.36	0.54
1:J:317:LYS:HE2	1:L:261:ASN:HB2	1.91	0.53
1:B:175:MET:O	1:B:249:ASN:ND2	2.41	0.53
1:C:261:ASN:HB2	1:E:317:LYS:HE2	1.91	0.53
1:H:317:LYS:HE2	1:J:261:ASN:HB2	1.90	0.53
1:I:261:ASN:HB2	1:K:317:LYS:HE2	1.90	0.53
1:K:307:PHE:N	1:K:314:PHE:O	2.36	0.53
1:L:317:LYS:HE2	1:N:261:ASN:HB2	1.91	0.53
1:W:261:ASN:HB2	1:Y:317:LYS:HE2	1.91	0.53
1:E:261:ASN:HB2	1:G:317:LYS:HE2	1.91	0.53
2:K:401:ATP:O1A	1:M:110:PHE:N	2.34	0.53
1:K:261:ASN:HB2	1:M:317:LYS:HE2	1.91	0.53
1:G:261:ASN:HB2	1:I:317:LYS:HE2	1.91	0.53
1:U:261:ASN:HB2	1:W:317:LYS:HE2	1.91	0.53
1:V:317:LYS:HE2	1:X:261:ASN:HB2	1.91	0.53
1:N:317:LYS:HE2	1:P:261:ASN:HB2	1.91	0.53
1:F:317:LYS:HE2	1:H:261:ASN:HB2	1.91	0.53
2:Q:401:ATP:O1A	1:S:110:PHE:N	2.34	0.53
1:A:261:ASN:HB2	1:C:317:LYS:HE2	1.91	0.53
1:D:317:LYS:HE2	1:F:261:ASN:HB2	1.90	0.53
1:S:261:ASN:HB2	1:U:317:LYS:HE2	1.91	0.53
1:J:110:PHE:N	2:L:401:ATP:O1A	2.34	0.53
1:M:261:ASN:HB2	1:O:317:LYS:HE2	1.91	0.53
1:Q:261:ASN:HB2	1:S:317:LYS:HE2	1.91	0.52
1:S:175:MET:O	1:S:249:ASN:ND2	2.41	0.52
1:T:317:LYS:HE2	1:V:261:ASN:HB2	1.90	0.52
1:B:317:LYS:HE2	1:D:261:ASN:HB2	1.91	0.52
1:P:317:LYS:HE2	1:R:261:ASN:HB2	1.91	0.52
1:A:317:LYS:HE2	1:B:261:ASN:HB2	1.91	0.52
1:N:110:PHE:N	2:P:401:ATP:O1A	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:261:ASN:HB2	1:Q:317:LYS:HE2	1.91	0.52
1:P:175:MET:O	1:P:249:ASN:ND2	2.41	0.52
1:L:175:MET:O	1:L:249:ASN:ND2	2.41	0.52
1:P:152:GLN:HE21	1:P:182:ALA:HB1	1.75	0.52
1:R:317:LYS:HE2	1:T:261:ASN:HB2	1.90	0.52
1:C:152:GLN:HE21	1:C:182:ALA:HB1	1.75	0.52
1:A:152:GLN:HE21	1:A:182:ALA:HB1	1.75	0.52
1:F:110:PHE:N	2:H:401:ATP:O1A	2.34	0.52
1:H:175:MET:O	1:H:249:ASN:ND2	2.41	0.52
1:K:175:MET:O	1:K:249:ASN:ND2	2.41	0.52
1:M:152:GLN:HE21	1:M:182:ALA:HB1	1.75	0.52
1:N:152:GLN:HE21	1:N:182:ALA:HB1	1.75	0.52
1:S:152:GLN:HE21	1:S:182:ALA:HB1	1.75	0.52
1:X:175:MET:O	1:X:249:ASN:ND2	2.41	0.52
1:E:175:MET:O	1:E:249:ASN:ND2	2.41	0.52
1:F:152:GLN:HE21	1:F:182:ALA:HB1	1.75	0.52
1:K:152:GLN:HE21	1:K:182:ALA:HB1	1.75	0.52
1:O:175:MET:O	1:O:249:ASN:ND2	2.41	0.52
1:R:152:GLN:HE21	1:R:182:ALA:HB1	1.75	0.52
1:W:175:MET:O	1:W:249:ASN:ND2	2.41	0.52
1:D:152:GLN:HE21	1:D:182:ALA:HB1	1.75	0.52
1:F:175:MET:O	1:F:249:ASN:ND2	2.41	0.51
1:I:175:MET:O	1:I:249:ASN:ND2	2.41	0.51
1:O:152:GLN:HE21	1:O:182:ALA:HB1	1.75	0.51
1:V:152:GLN:HE21	1:V:182:ALA:HB1	1.75	0.51
1:X:152:GLN:HE21	1:X:182:ALA:HB1	1.75	0.51
1:H:152:GLN:HE21	1:H:182:ALA:HB1	1.75	0.51
1:Q:152:GLN:HE21	1:Q:182:ALA:HB1	1.75	0.51
1:T:175:MET:O	1:T:249:ASN:ND2	2.41	0.51
1:E:152:GLN:HE21	1:E:182:ALA:HB1	1.75	0.51
2:G:401:ATP:O1A	1:I:110:PHE:N	2.34	0.51
1:L:152:GLN:HE21	1:L:182:ALA:HB1	1.75	0.51
1:U:152:GLN:HE21	1:U:182:ALA:HB1	1.75	0.51
1:B:152:GLN:HE21	1:B:182:ALA:HB1	1.75	0.51
2:W:401:ATP:O1A	1:Y:110:PHE:N	2.34	0.51
1:I:152:GLN:HE21	1:I:182:ALA:HB1	1.75	0.51
1:T:152:GLN:HE21	1:T:182:ALA:HB1	1.75	0.51
1:V:175:MET:O	1:V:249:ASN:ND2	2.41	0.51
1:M:175:MET:O	1:M:249:ASN:ND2	2.41	0.51
1:Y:175:MET:O	1:Y:249:ASN:ND2	2.41	0.51
1:J:175:MET:O	1:J:249:ASN:ND2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:295:ASP:O	1:Q:298:SER:OG	2.21	0.51
1:R:295:ASP:O	1:R:298:SER:OG	2.21	0.51
1:T:212:GLU:O	1:T:215:THR:OG1	2.29	0.51
1:Y:152:GLN:HE21	1:Y:182:ALA:HB1	1.75	0.51
1:J:152:GLN:HE21	1:J:182:ALA:HB1	1.75	0.51
1:F:212:GLU:O	1:F:215:THR:OG1	2.29	0.51
1:G:152:GLN:HE21	1:G:182:ALA:HB1	1.75	0.50
1:W:104:THR:OG1	1:W:105:GLY:N	2.44	0.50
1:Y:104:THR:OG1	1:Y:105:GLY:N	2.44	0.50
1:D:212:GLU:O	1:D:215:THR:OG1	2.29	0.50
1:W:152:GLN:HE21	1:W:182:ALA:HB1	1.75	0.50
1:A:212:GLU:O	1:A:215:THR:OG1	2.29	0.50
1:V:104:THR:OG1	1:V:105:GLY:N	2.44	0.50
1:B:212:GLU:O	1:B:215:THR:OG1	2.29	0.50
1:B:295:ASP:O	1:B:298:SER:OG	2.21	0.50
1:D:175:MET:O	1:D:249:ASN:ND2	2.41	0.50
1:T:104:THR:OG1	1:T:105:GLY:N	2.44	0.50
1:X:104:THR:OG1	1:X:105:GLY:N	2.44	0.50
1:A:175:MET:O	1:A:249:ASN:ND2	2.41	0.50
1:G:104:THR:OG1	1:G:105:GLY:N	2.44	0.50
1:G:175:MET:O	1:G:249:ASN:ND2	2.41	0.50
1:K:212:GLU:O	1:K:215:THR:OG1	2.29	0.50
1:M:104:THR:OG1	1:M:105:GLY:N	2.44	0.50
1:O:104:THR:OG1	1:O:105:GLY:N	2.44	0.50
1:S:170:ASP:OD1	1:S:171:GLU:N	2.44	0.50
1:U:104:THR:OG1	1:U:105:GLY:N	2.44	0.50
1:U:170:ASP:OD1	1:U:171:GLU:N	2.44	0.50
1:M:212:GLU:O	1:M:215:THR:OG1	2.29	0.50
1:E:104:THR:OG1	1:E:105:GLY:N	2.44	0.50
1:Q:104:THR:OG1	1:Q:105:GLY:N	2.44	0.50
1:C:170:ASP:OD1	1:C:171:GLU:N	2.44	0.50
1:D:255:SER:HA	1:D:258:ILE:HG22	1.94	0.50
1:F:255:SER:HA	1:F:258:ILE:HG22	1.94	0.50
1:N:255:SER:HA	1:N:258:ILE:HG22	1.94	0.50
1:O:212:GLU:O	1:O:215:THR:OG1	2.29	0.50
1:R:104:THR:OG1	1:R:105:GLY:N	2.44	0.50
1:S:104:THR:OG1	1:S:105:GLY:N	2.44	0.50
1:V:255:SER:HA	1:V:258:ILE:HG22	1.94	0.50
1:D:104:THR:OG1	1:D:105:GLY:N	2.44	0.50
1:F:104:THR:OG1	1:F:105:GLY:N	2.44	0.50
1:H:104:THR:OG1	1:H:105:GLY:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:104:THR:OG1	1:J:105:GLY:N	2.44	0.50
1:L:104:THR:OG1	1:L:105:GLY:N	2.44	0.50
1:L:255:SER:HA	1:L:258:ILE:HG22	1.94	0.50
1:Q:212:GLU:O	1:Q:215:THR:OG1	2.29	0.50
1:S:255:SER:HA	1:S:258:ILE:HG22	1.94	0.50
1:T:255:SER:HA	1:T:258:ILE:HG22	1.94	0.50
1:U:255:SER:HA	1:U:258:ILE:HG22	1.94	0.50
1:W:170:ASP:OD1	1:W:171:GLU:N	2.45	0.50
1:X:255:SER:HA	1:X:258:ILE:HG22	1.94	0.50
1:A:170:ASP:OD1	1:A:171:GLU:N	2.44	0.49
1:B:255:SER:HA	1:B:258:ILE:HG22	1.94	0.49
1:E:170:ASP:OD1	1:E:171:GLU:N	2.45	0.49
1:N:104:THR:OG1	1:N:105:GLY:N	2.44	0.49
1:Q:170:ASP:OD1	1:Q:171:GLU:N	2.44	0.49
1:Q:255:SER:HA	1:Q:258:ILE:HG22	1.94	0.49
1:B:104:THR:OG1	1:B:105:GLY:N	2.44	0.49
1:C:104:THR:OG1	1:C:105:GLY:N	2.44	0.49
1:D:184:LYS:NZ	1:D:256:SER:O	2.46	0.49
1:E:255:SER:HA	1:E:258:ILE:HG22	1.94	0.49
1:H:255:SER:HA	1:H:258:ILE:HG22	1.94	0.49
1:O:255:SER:HA	1:O:258:ILE:HG22	1.94	0.49
1:P:104:THR:OG1	1:P:105:GLY:N	2.44	0.49
1:R:255:SER:HA	1:R:258:ILE:HG22	1.94	0.49
1:S:212:GLU:O	1:S:215:THR:OG1	2.29	0.49
1:W:255:SER:HA	1:W:258:ILE:HG22	1.94	0.49
1:A:255:SER:HA	1:A:258:ILE:HG22	1.94	0.49
1:F:184:LYS:NZ	1:F:256:SER:O	2.46	0.49
1:G:255:SER:HA	1:G:258:ILE:HG22	1.94	0.49
1:J:255:SER:HA	1:J:258:ILE:HG22	1.94	0.49
1:N:170:ASP:OD1	1:N:171:GLU:N	2.44	0.49
1:R:175:MET:O	1:R:249:ASN:ND2	2.41	0.49
1:Y:255:SER:HA	1:Y:258:ILE:HG22	1.94	0.49
1:A:104:THR:OG1	1:A:105:GLY:N	2.44	0.49
1:H:184:LYS:NZ	1:H:256:SER:O	2.46	0.49
1:M:255:SER:HA	1:M:258:ILE:HG22	1.94	0.49
1:O:295:ASP:O	1:O:298:SER:OG	2.21	0.49
1:P:170:ASP:OD1	1:P:171:GLU:N	2.44	0.49
1:P:255:SER:HA	1:P:258:ILE:HG22	1.94	0.49
2:S:401:ATP:O1A	1:U:110:PHE:N	2.34	0.49
1:C:255:SER:HA	1:C:258:ILE:HG22	1.94	0.49
1:G:170:ASP:OD1	1:G:171:GLU:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:255:SER:HA	1:I:258:ILE:HG22	1.94	0.49
1:K:255:SER:HA	1:K:258:ILE:HG22	1.94	0.49
1:Y:212:GLU:O	1:Y:215:THR:OG1	2.29	0.49
2:E:401:ATP:O1A	1:G:110:PHE:N	2.34	0.49
1:J:184:LYS:NZ	1:J:256:SER:O	2.46	0.49
1:Q:175:MET:O	1:Q:249:ASN:ND2	2.41	0.49
1:T:295:ASP:O	1:T:298:SER:OG	2.21	0.49
1:Y:170:ASP:OD1	1:Y:171:GLU:N	2.44	0.49
1:E:184:LYS:NZ	1:E:256:SER:O	2.46	0.49
1:I:104:THR:OG1	1:I:105:GLY:N	2.44	0.49
1:K:104:THR:OG1	1:K:105:GLY:N	2.44	0.49
1:L:170:ASP:OD1	1:L:171:GLU:N	2.44	0.49
1:Q:184:LYS:NZ	1:Q:256:SER:O	2.46	0.49
1:U:175:MET:O	1:U:249:ASN:ND2	2.41	0.49
1:B:170:ASP:OD1	1:B:171:GLU:N	2.44	0.49
1:O:170:ASP:OD1	1:O:171:GLU:N	2.44	0.49
1:R:170:ASP:OD1	1:R:171:GLU:N	2.44	0.49
1:I:170:ASP:OD1	1:I:171:GLU:N	2.44	0.49
1:K:170:ASP:OD1	1:K:171:GLU:N	2.44	0.49
1:P:184:LYS:NZ	1:P:256:SER:O	2.46	0.49
1:N:175:MET:O	1:N:249:ASN:ND2	2.41	0.48
1:R:184:LYS:NZ	1:R:256:SER:O	2.46	0.48
2:U:401:ATP:O1A	1:W:110:PHE:N	2.34	0.48
1:A:242:VAL:O	1:A:246:ASN:N	2.47	0.48
1:R:242:VAL:O	1:R:246:ASN:N	2.47	0.48
1:S:242:VAL:O	1:S:246:ASN:N	2.47	0.48
1:N:295:ASP:O	1:N:298:SER:OG	2.21	0.48
1:X:113:LYS:NZ	1:X:117:GLU:OE2	2.45	0.48
1:C:184:LYS:NZ	1:C:256:SER:O	2.46	0.48
1:C:242:VAL:O	1:C:246:ASN:N	2.47	0.48
1:J:170:ASP:OD1	1:J:171:GLU:N	2.44	0.48
1:L:110:PHE:N	2:N:401:ATP:O1A	2.33	0.48
1:M:170:ASP:OD1	1:M:171:GLU:N	2.44	0.48
1:M:184:LYS:NZ	1:M:256:SER:O	2.46	0.48
1:U:295:ASP:O	1:U:298:SER:OG	2.21	0.48
1:H:242:VAL:O	1:H:246:ASN:N	2.47	0.48
1:P:242:VAL:O	1:P:246:ASN:N	2.47	0.48
1:U:242:VAL:O	1:U:246:ASN:N	2.47	0.48
1:G:242:VAL:O	1:G:246:ASN:N	2.47	0.48
1:H:170:ASP:OD1	1:H:171:GLU:N	2.45	0.48
1:L:242:VAL:O	1:L:246:ASN:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:242:VAL:O	1:Q:246:ASN:N	2.47	0.48
1:B:242:VAL:O	1:B:246:ASN:N	2.47	0.48
1:D:295:ASP:O	1:D:298:SER:OG	2.21	0.48
1:K:242:VAL:O	1:K:246:ASN:N	2.47	0.48
1:L:184:LYS:NZ	1:L:256:SER:O	2.46	0.48
1:M:242:VAL:O	1:M:246:ASN:N	2.47	0.48
1:T:184:LYS:NZ	1:T:256:SER:O	2.46	0.48
1:X:110:PHE:N	2:X:402:ATP:O1A	2.33	0.48
1:F:170:ASP:OD1	1:F:171:GLU:N	2.44	0.48
1:K:184:LYS:NZ	1:K:256:SER:O	2.46	0.48
1:T:170:ASP:OD1	1:T:171:GLU:N	2.44	0.48
1:Y:242:VAL:O	1:Y:246:ASN:N	2.47	0.48
1:D:170:ASP:OD1	1:D:171:GLU:N	2.44	0.48
1:I:242:VAL:O	1:I:246:ASN:N	2.47	0.48
1:J:242:VAL:O	1:J:246:ASN:N	2.47	0.48
1:L:212:GLU:O	1:L:215:THR:OG1	2.29	0.48
1:T:242:VAL:O	1:T:246:ASN:N	2.47	0.48
1:V:242:VAL:O	1:V:246:ASN:N	2.47	0.48
1:F:242:VAL:O	1:F:246:ASN:N	2.47	0.48
1:N:212:GLU:O	1:N:215:THR:OG1	2.29	0.47
1:D:242:VAL:O	1:D:246:ASN:N	2.47	0.47
1:X:242:VAL:O	1:X:246:ASN:N	2.47	0.47
1:E:212:GLU:O	1:E:215:THR:OG1	2.29	0.47
1:H:110:PHE:N	2:J:401:ATP:O1A	2.33	0.47
1:I:184:LYS:NZ	1:I:256:SER:O	2.46	0.47
1:N:184:LYS:NZ	1:N:256:SER:O	2.46	0.47
1:N:242:VAL:O	1:N:246:ASN:N	2.47	0.47
1:O:242:VAL:O	1:O:246:ASN:N	2.47	0.47
1:U:184:LYS:NZ	1:U:256:SER:O	2.46	0.47
1:V:184:LYS:NZ	1:V:256:SER:O	2.46	0.47
1:E:242:VAL:O	1:E:246:ASN:N	2.47	0.47
1:W:242:VAL:O	1:W:246:ASN:N	2.47	0.47
1:X:170:ASP:OD1	1:X:171:GLU:N	2.44	0.47
1:A:184:LYS:NZ	1:A:256:SER:O	2.46	0.47
1:G:212:GLU:O	1:G:215:THR:OG1	2.29	0.47
1:J:113:LYS:NZ	1:J:117:GLU:OE2	2.45	0.47
1:J:212:GLU:O	1:J:215:THR:OG1	2.29	0.47
1:T:84:PHE:O	1:T:88:ASN:ND2	2.48	0.47
1:D:84:PHE:O	1:D:88:ASN:ND2	2.48	0.47
1:E:295:ASP:O	1:E:298:SER:OG	2.21	0.47
1:L:84:PHE:O	1:L:88:ASN:ND2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:84:PHE:O	1:R:88:ASN:ND2	2.48	0.47
1:V:84:PHE:O	1:V:88:ASN:ND2	2.48	0.47
1:V:170:ASP:OD1	1:V:171:GLU:N	2.44	0.47
1:M:84:PHE:O	1:M:88:ASN:ND2	2.48	0.47
1:N:84:PHE:O	1:N:88:ASN:ND2	2.48	0.47
1:P:84:PHE:O	1:P:88:ASN:ND2	2.48	0.47
1:B:84:PHE:O	1:B:88:ASN:ND2	2.48	0.47
1:M:295:ASP:O	1:M:298:SER:OG	2.21	0.47
1:V:113:LYS:NZ	1:V:117:GLU:OE2	2.45	0.47
1:W:212:GLU:O	1:W:215:THR:OG1	2.29	0.47
1:A:84:PHE:O	1:A:88:ASN:ND2	2.48	0.47
1:B:113:LYS:NZ	1:B:117:GLU:OE2	2.45	0.47
1:C:84:PHE:O	1:C:88:ASN:ND2	2.48	0.47
1:C:212:GLU:O	1:C:215:THR:OG1	2.29	0.47
1:E:84:PHE:O	1:E:88:ASN:ND2	2.48	0.47
1:O:84:PHE:O	1:O:88:ASN:ND2	2.48	0.47
1:V:295:ASP:O	1:V:298:SER:OG	2.21	0.47
1:X:184:LYS:NZ	1:X:256:SER:O	2.46	0.47
1:A:104:THR:HG1	2:B:401:ATP:PG	2.38	0.46
1:S:113:LYS:NZ	1:S:117:GLU:OE2	2.45	0.46
1:G:84:PHE:O	1:G:88:ASN:ND2	2.48	0.46
2:I:401:ATP:O1A	1:K:110:PHE:N	2.33	0.46
1:J:84:PHE:O	1:J:88:ASN:ND2	2.48	0.46
1:Q:84:PHE:O	1:Q:88:ASN:ND2	2.48	0.46
1:U:212:GLU:O	1:U:215:THR:OG1	2.29	0.46
1:W:84:PHE:O	1:W:88:ASN:ND2	2.48	0.46
1:P:212:GLU:O	1:P:215:THR:OG1	2.29	0.46
1:U:84:PHE:O	1:U:88:ASN:ND2	2.48	0.46
1:E:113:LYS:NZ	1:E:117:GLU:OE2	2.45	0.46
1:G:184:LYS:NZ	1:G:256:SER:O	2.46	0.46
1:S:84:PHE:O	1:S:88:ASN:ND2	2.48	0.46
1:H:113:LYS:NZ	1:H:117:GLU:OE2	2.45	0.46
1:B:184:LYS:NZ	1:B:256:SER:O	2.46	0.46
1:I:212:GLU:O	1:I:215:THR:OG1	2.29	0.46
1:L:295:ASP:O	1:L:298:SER:OG	2.21	0.46
2:C:401:ATP:PG	1:E:104:THR:HG1	2.39	0.46
1:K:233:LEU:HD23	1:M:328:TYR:CE1	2.51	0.46
2:Q:401:ATP:PG	1:S:104:THR:HG1	2.39	0.46
1:Y:84:PHE:O	1:Y:88:ASN:ND2	2.48	0.46
1:C:233:LEU:HD23	1:E:328:TYR:CE1	2.51	0.46
1:E:233:LEU:HD23	1:G:328:TYR:CE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:328:TYR:CE1	1:H:233:LEU:HD23	2.51	0.46
1:G:233:LEU:HD23	1:I:328:TYR:CE1	2.51	0.46
1:M:233:LEU:HD23	1:O:328:TYR:CE1	2.51	0.46
1:U:233:LEU:HD23	1:W:328:TYR:CE1	2.51	0.46
1:W:295:ASP:O	1:W:298:SER:OG	2.21	0.46
1:H:212:GLU:O	1:H:215:THR:OG1	2.29	0.45
1:I:233:LEU:HD23	1:K:328:TYR:CE1	2.52	0.45
1:J:328:TYR:CE1	1:L:233:LEU:HD23	2.51	0.45
1:V:328:TYR:CE1	1:X:233:LEU:HD23	2.51	0.45
1:F:295:ASP:O	1:F:298:SER:OG	2.21	0.45
1:G:295:ASP:O	1:G:298:SER:OG	2.21	0.45
1:I:84:PHE:O	1:I:88:ASN:ND2	2.48	0.45
1:T:328:TYR:CE1	1:V:233:LEU:HD23	2.51	0.45
1:L:328:TYR:CE1	1:N:233:LEU:HD23	2.51	0.45
1:A:233:LEU:HD23	1:C:328:TYR:CE1	2.51	0.45
1:O:113:LYS:NZ	1:O:117:GLU:OE2	2.45	0.45
1:O:233:LEU:HD23	1:Q:328:TYR:CE1	2.51	0.45
1:A:328:TYR:CE1	1:B:233:LEU:HD23	2.51	0.45
1:P:113:LYS:NZ	1:P:117:GLU:OE2	2.45	0.45
1:S:184:LYS:NZ	1:S:256:SER:O	2.46	0.45
1:D:328:TYR:CE1	1:F:233:LEU:HD23	2.51	0.45
1:O:184:LYS:NZ	1:O:256:SER:O	2.46	0.45
1:R:113:LYS:NZ	1:R:117:GLU:OE2	2.45	0.45
1:X:212:GLU:O	1:X:215:THR:OG1	2.29	0.45
1:B:328:TYR:CE1	1:D:233:LEU:HD23	2.51	0.45
1:F:84:PHE:O	1:F:88:ASN:ND2	2.48	0.45
1:H:84:PHE:O	1:H:88:ASN:ND2	2.48	0.45
1:H:328:TYR:CE1	1:J:233:LEU:HD23	2.51	0.45
1:Q:233:LEU:HD23	1:S:328:TYR:CE1	2.51	0.45
1:R:328:TYR:CE1	1:T:233:LEU:HD23	2.51	0.45
1:S:233:LEU:HD23	1:U:328:TYR:CE1	2.51	0.45
1:K:295:ASP:O	1:K:298:SER:OG	2.21	0.44
1:N:113:LYS:NZ	1:N:117:GLU:OE2	2.45	0.44
1:W:233:LEU:HD23	1:Y:328:TYR:CE1	2.51	0.44
1:P:104:THR:HG1	2:R:401:ATP:PG	2.40	0.44
1:R:212:GLU:O	1:R:215:THR:OG1	2.29	0.44
1:X:84:PHE:O	1:X:88:ASN:ND2	2.48	0.44
1:X:295:ASP:O	1:X:298:SER:OG	2.21	0.44
1:P:328:TYR:CE1	1:R:233:LEU:HD23	2.51	0.44
1:G:113:LYS:NZ	1:G:117:GLU:OE2	2.45	0.44
1:N:328:TYR:CE1	1:P:233:LEU:HD23	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:113:LYS:NZ	1:F:117:GLU:OE2	2.45	0.44
1:J:295:ASP:O	1:J:298:SER:OG	2.21	0.44
1:K:84:PHE:O	1:K:88:ASN:ND2	2.48	0.44
1:U:113:LYS:NZ	1:U:117:GLU:OE2	2.45	0.44
1:H:295:ASP:O	1:H:298:SER:OG	2.21	0.44
1:Y:184:LYS:NZ	1:Y:256:SER:O	2.46	0.44
1:Y:295:ASP:O	1:Y:298:SER:OG	2.21	0.44
1:P:283:VAL:O	1:P:287:SER:OG	2.34	0.44
1:Y:113:LYS:NZ	1:Y:117:GLU:OE2	2.45	0.44
1:I:295:ASP:O	1:I:298:SER:OG	2.21	0.43
1:V:212:GLU:O	1:V:215:THR:OG1	2.29	0.43
1:M:113:LYS:NZ	1:M:117:GLU:OE2	2.45	0.43
1:T:113:LYS:NZ	1:T:117:GLU:OE2	2.45	0.43
1:I:113:LYS:NZ	1:I:117:GLU:OE2	2.45	0.42
1:B:97:THR:OG1	1:B:264:ASP:N	2.53	0.42
1:G:97:THR:OG1	1:G:264:ASP:N	2.53	0.42
1:H:97:THR:OG1	1:H:264:ASP:N	2.53	0.42
1:I:97:THR:OG1	1:I:264:ASP:N	2.53	0.42
1:K:97:THR:OG1	1:K:264:ASP:N	2.53	0.42
1:O:97:THR:OG1	1:O:264:ASP:N	2.53	0.42
1:T:97:THR:OG1	1:T:264:ASP:N	2.53	0.42
1:W:97:THR:OG1	1:W:264:ASP:N	2.53	0.42
1:Y:97:THR:OG1	1:Y:264:ASP:N	2.53	0.42
1:A:113:LYS:NZ	1:A:117:GLU:OE2	2.45	0.42
1:D:97:THR:OG1	1:D:264:ASP:N	2.53	0.42
1:E:97:THR:OG1	1:E:264:ASP:N	2.53	0.42
1:F:97:THR:OG1	1:F:264:ASP:N	2.53	0.42
1:J:97:THR:OG1	1:J:264:ASP:N	2.53	0.42
1:L:97:THR:OG1	1:L:264:ASP:N	2.53	0.42
1:M:97:THR:OG1	1:M:264:ASP:N	2.53	0.42
1:N:104:THR:HG1	2:P:401:ATP:PG	2.42	0.42
1:R:97:THR:OG1	1:R:264:ASP:N	2.53	0.42
1:X:97:THR:OG1	1:X:264:ASP:N	2.53	0.42
1:V:97:THR:OG1	1:V:264:ASP:N	2.53	0.42
1:Q:97:THR:OG1	1:Q:264:ASP:N	2.53	0.42
1:U:97:THR:OG1	1:U:264:ASP:N	2.53	0.42
1:D:221:PHE:O	1:D:224:SER:OG	2.35	0.42
1:A:97:THR:OG1	1:A:264:ASP:N	2.53	0.42
2:O:401:ATP:PG	1:Q:104:THR:HG1	2.42	0.42
1:N:97:THR:OG1	1:N:264:ASP:N	2.53	0.42
1:U:283:VAL:O	1:U:287:SER:OG	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:97:THR:OG1	1:P:264:ASP:N	2.53	0.42
1:E:252:PHE:O	1:E:255:SER:OG	2.21	0.41
1:C:97:THR:OG1	1:C:264:ASP:N	2.53	0.41
1:S:97:THR:OG1	1:S:264:ASP:N	2.53	0.41
2:U:401:ATP:PG	1:W:104:THR:HG1	2.43	0.41
1:R:104:THR:HG1	2:T:401:ATP:PG	2.43	0.41
1:W:113:LYS:NZ	1:W:117:GLU:OE2	2.45	0.41
1:W:184:LYS:NZ	1:W:256:SER:O	2.46	0.41
1:W:283:VAL:O	1:W:287:SER:OG	2.34	0.41
1:D:113:LYS:NZ	1:D:117:GLU:OE2	2.45	0.40
1:H:221:PHE:O	1:H:224:SER:OG	2.34	0.40
1:K:113:LYS:NZ	1:K:117:GLU:OE2	2.45	0.40
1:X:134:ALA:O	1:X:138:PHE:N	2.50	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	280/282 (99%)	248 (89%)	32 (11%)	0	100	100
1	B	280/282 (99%)	248 (89%)	32 (11%)	0	100	100
1	C	280/282 (99%)	248 (89%)	32 (11%)	0	100	100
1	D	280/282 (99%)	248 (89%)	32 (11%)	0	100	100
1	E	280/282 (99%)	248 (89%)	32 (11%)	0	100	100
1	F	280/282 (99%)	248 (89%)	32 (11%)	0	100	100
1	G	280/282 (99%)	248 (89%)	32 (11%)	0	100	100
1	H	280/282 (99%)	248 (89%)	32 (11%)	0	100	100
1	I	280/282 (99%)	248 (89%)	32 (11%)	0	100	100
1	J	280/282 (99%)	248 (89%)	32 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	280/282 (99%)	248 (89%)	32 (11%)	0	100	100
1	L	280/282 (99%)	248 (89%)	32 (11%)	0	100	100
1	M	280/282 (99%)	248 (89%)	32 (11%)	0	100	100
1	N	280/282 (99%)	248 (89%)	32 (11%)	0	100	100
1	O	280/282 (99%)	248 (89%)	32 (11%)	0	100	100
1	P	280/282 (99%)	248 (89%)	32 (11%)	0	100	100
1	Q	280/282 (99%)	247 (88%)	33 (12%)	0	100	100
1	R	280/282 (99%)	248 (89%)	32 (11%)	0	100	100
1	S	280/282 (99%)	248 (89%)	32 (11%)	0	100	100
1	T	280/282 (99%)	248 (89%)	32 (11%)	0	100	100
1	U	280/282 (99%)	248 (89%)	32 (11%)	0	100	100
1	V	280/282 (99%)	248 (89%)	32 (11%)	0	100	100
1	W	280/282 (99%)	248 (89%)	32 (11%)	0	100	100
1	X	280/282 (99%)	248 (89%)	32 (11%)	0	100	100
1	Y	280/282 (99%)	248 (89%)	32 (11%)	0	100	100
All	All	7000/7050 (99%)	6199 (89%)	801 (11%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	250/250 (100%)	250 (100%)	0	100	100
1	B	250/250 (100%)	250 (100%)	0	100	100
1	C	250/250 (100%)	250 (100%)	0	100	100
1	D	250/250 (100%)	250 (100%)	0	100	100
1	E	250/250 (100%)	250 (100%)	0	100	100
1	F	250/250 (100%)	250 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	250/250 (100%)	250 (100%)	0	100	100
1	H	250/250 (100%)	250 (100%)	0	100	100
1	I	250/250 (100%)	250 (100%)	0	100	100
1	J	250/250 (100%)	250 (100%)	0	100	100
1	K	250/250 (100%)	250 (100%)	0	100	100
1	L	250/250 (100%)	250 (100%)	0	100	100
1	M	250/250 (100%)	250 (100%)	0	100	100
1	N	250/250 (100%)	250 (100%)	0	100	100
1	O	250/250 (100%)	250 (100%)	0	100	100
1	P	250/250 (100%)	250 (100%)	0	100	100
1	Q	250/250 (100%)	250 (100%)	0	100	100
1	R	250/250 (100%)	250 (100%)	0	100	100
1	S	250/250 (100%)	250 (100%)	0	100	100
1	T	250/250 (100%)	250 (100%)	0	100	100
1	U	250/250 (100%)	250 (100%)	0	100	100
1	V	250/250 (100%)	250 (100%)	0	100	100
1	W	250/250 (100%)	250 (100%)	0	100	100
1	X	250/250 (100%)	250 (100%)	0	100	100
1	Y	250/250 (100%)	250 (100%)	0	100	100
All	All	6250/6250 (100%)	6250 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (138) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	73	HIS
1	A	130	HIS
1	A	137	HIS
1	A	152	GLN
1	B	72	GLN
1	B	73	HIS
1	B	130	HIS
1	B	137	HIS

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Mol	Chain	Res	Type
1	B	152	GLN
1	B	238	HIS
1	C	72	GLN
1	C	73	HIS
1	C	130	HIS
1	C	137	HIS
1	C	152	GLN
1	D	72	GLN
1	D	73	HIS
1	D	130	HIS
1	D	137	HIS
1	D	152	GLN
1	D	238	HIS
1	E	72	GLN
1	E	73	HIS
1	E	130	HIS
1	E	137	HIS
1	E	152	GLN
1	E	238	HIS
1	F	72	GLN
1	F	73	HIS
1	F	130	HIS
1	F	137	HIS
1	F	152	GLN
1	F	238	HIS
1	G	72	GLN
1	G	73	HIS
1	G	130	HIS
1	G	137	HIS
1	G	152	GLN
1	G	238	HIS
1	H	72	GLN
1	H	73	HIS
1	H	130	HIS
1	H	137	HIS
1	H	152	GLN
1	H	238	HIS
1	I	72	GLN
1	I	73	HIS
1	I	130	HIS
1	I	137	HIS
1	I	152	GLN

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Mol	Chain	Res	Type
1	I	238	HIS
1	J	72	GLN
1	J	73	HIS
1	J	130	HIS
1	J	137	HIS
1	J	152	GLN
1	K	72	GLN
1	K	73	HIS
1	K	130	HIS
1	K	137	HIS
1	K	152	GLN
1	K	238	HIS
1	L	72	GLN
1	L	73	HIS
1	L	130	HIS
1	L	137	HIS
1	L	152	GLN
1	L	238	HIS
1	M	72	GLN
1	M	73	HIS
1	M	130	HIS
1	M	137	HIS
1	M	152	GLN
1	N	72	GLN
1	N	73	HIS
1	N	130	HIS
1	N	137	HIS
1	N	152	GLN
1	O	72	GLN
1	O	137	HIS
1	O	152	GLN
1	O	238	HIS
1	P	72	GLN
1	P	73	HIS
1	P	130	HIS
1	P	137	HIS
1	P	152	GLN
1	Q	72	GLN
1	Q	73	HIS
1	Q	130	HIS
1	Q	137	HIS
1	Q	152	GLN

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Mol	Chain	Res	Type
1	Q	238	HIS
1	R	72	GLN
1	R	73	HIS
1	R	130	HIS
1	R	137	HIS
1	R	152	GLN
1	R	238	HIS
1	S	72	GLN
1	S	73	HIS
1	S	130	HIS
1	S	137	HIS
1	S	152	GLN
1	S	238	HIS
1	T	72	GLN
1	T	73	HIS
1	T	130	HIS
1	T	137	HIS
1	T	152	GLN
1	T	238	HIS
1	U	72	GLN
1	U	73	HIS
1	U	130	HIS
1	U	137	HIS
1	U	152	GLN
1	V	72	GLN
1	V	73	HIS
1	V	130	HIS
1	V	137	HIS
1	V	152	GLN
1	W	72	GLN
1	W	73	HIS
1	W	130	HIS
1	W	137	HIS
1	W	152	GLN
1	W	238	HIS
1	X	72	GLN
1	X	73	HIS
1	X	130	HIS
1	X	137	HIS
1	X	152	GLN
1	Y	72	GLN
1	Y	73	HIS

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Mol	Chain	Res	Type
1	Y	130	HIS
1	Y	137	HIS
1	Y	152	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

25 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	$\# Z > 2$
2	ATP	B	401	-	32,33,33	1.29	5 (15%)	48,52,52	1.80	9 (18%)
2	ATP	J	401	-	32,33,33	1.29	5 (15%)	48,52,52	1.81	9 (18%)
2	ATP	H	401	-	32,33,33	1.29	5 (15%)	48,52,52	1.80	9 (18%)
2	ATP	G	401	-	32,33,33	1.29	5 (15%)	48,52,52	1.81	9 (18%)
2	ATP	X	401	-	32,33,33	1.30	5 (15%)	48,52,52	1.81	9 (18%)
2	ATP	A	401	-	32,33,33	1.29	5 (15%)	48,52,52	1.80	9 (18%)
2	ATP	S	401	-	32,33,33	1.29	5 (15%)	48,52,52	1.81	9 (18%)
2	ATP	Q	401	-	32,33,33	1.29	5 (15%)	48,52,52	1.80	9 (18%)
2	ATP	N	401	-	32,33,33	1.30	5 (15%)	48,52,52	1.81	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ATP	X	402	-	32,33,33	1.29	5 (15%)	48,52,52	1.81	9 (18%)
2	ATP	T	401	-	32,33,33	1.28	5 (15%)	48,52,52	1.81	9 (18%)
2	ATP	F	401	-	32,33,33	1.29	5 (15%)	48,52,52	1.80	9 (18%)
2	ATP	K	401	-	32,33,33	1.29	5 (15%)	48,52,52	1.80	9 (18%)
2	ATP	V	401	-	32,33,33	1.29	5 (15%)	48,52,52	1.81	9 (18%)
2	ATP	I	401	-	32,33,33	1.29	5 (15%)	48,52,52	1.81	9 (18%)
2	ATP	L	401	-	32,33,33	1.29	5 (15%)	48,52,52	1.80	9 (18%)
2	ATP	E	401	-	32,33,33	1.28	5 (15%)	48,52,52	1.80	9 (18%)
2	ATP	U	401	-	32,33,33	1.29	5 (15%)	48,52,52	1.80	9 (18%)
2	ATP	D	401	-	32,33,33	1.29	5 (15%)	48,52,52	1.80	9 (18%)
2	ATP	W	401	-	32,33,33	1.29	5 (15%)	48,52,52	1.80	9 (18%)
2	ATP	M	401	-	32,33,33	1.29	5 (15%)	48,52,52	1.81	9 (18%)
2	ATP	R	401	-	32,33,33	1.29	5 (15%)	48,52,52	1.81	9 (18%)
2	ATP	P	401	-	32,33,33	1.29	5 (15%)	48,52,52	1.81	9 (18%)
2	ATP	O	401	-	32,33,33	1.29	5 (15%)	48,52,52	1.81	9 (18%)
2	ATP	C	401	-	32,33,33	1.29	5 (15%)	48,52,52	1.80	9 (18%)

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
2	ATP	B	401	-	-	1/22/38/38	0/3/3/3
2	ATP	J	401	-	-	1/22/38/38	0/3/3/3
2	ATP	H	401	-	-	1/22/38/38	0/3/3/3
2	ATP	G	401	-	-	1/22/38/38	0/3/3/3
2	ATP	X	401	-	-	1/22/38/38	0/3/3/3
2	ATP	A	401	-	-	1/22/38/38	0/3/3/3
2	ATP	S	401	-	-	1/22/38/38	0/3/3/3
2	ATP	Q	401	-	-	1/22/38/38	0/3/3/3
2	ATP	N	401	-	-	1/22/38/38	0/3/3/3
2	ATP	X	402	-	-	1/22/38/38	0/3/3/3
2	ATP	T	401	-	-	1/22/38/38	0/3/3/3
2	ATP	F	401	-	-	1/22/38/38	0/3/3/3
2	ATP	K	401	-	-	1/22/38/38	0/3/3/3
2	ATP	V	401	-	-	1/22/38/38	0/3/3/3
2	ATP	I	401	-	-	1/22/38/38	0/3/3/3
2	ATP	L	401	-	-	1/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ATP	E	401	-	-	1/22/38/38	0/3/3/3
2	ATP	U	401	-	-	1/22/38/38	0/3/3/3
2	ATP	D	401	-	-	1/22/38/38	0/3/3/3
2	ATP	W	401	-	-	1/22/38/38	0/3/3/3
2	ATP	M	401	-	-	1/22/38/38	0/3/3/3
2	ATP	R	401	-	-	1/22/38/38	0/3/3/3
2	ATP	P	401	-	-	1/22/38/38	0/3/3/3
2	ATP	O	401	-	-	1/22/38/38	0/3/3/3
2	ATP	C	401	-	-	1/22/38/38	0/3/3/3

All (125) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	401	ATP	C5-C4	4.29	1.46	1.39
2	M	401	ATP	C5-C4	4.28	1.46	1.39
2	O	401	ATP	C5-C4	4.28	1.46	1.39
2	I	401	ATP	C5-C4	4.28	1.46	1.39
2	G	401	ATP	C5-C4	4.28	1.46	1.39
2	N	401	ATP	C5-C4	4.27	1.46	1.39
2	X	401	ATP	C5-C4	4.27	1.46	1.39
2	F	401	ATP	C5-C4	4.26	1.46	1.39
2	U	401	ATP	C5-C4	4.26	1.46	1.39
2	P	401	ATP	C5-C4	4.26	1.46	1.39
2	J	401	ATP	C5-C4	4.26	1.46	1.39
2	R	401	ATP	C5-C4	4.26	1.46	1.39
2	V	401	ATP	C5-C4	4.25	1.46	1.39
2	C	401	ATP	C5-C4	4.25	1.46	1.39
2	B	401	ATP	C5-C4	4.25	1.46	1.39
2	X	402	ATP	C5-C4	4.25	1.46	1.39
2	H	401	ATP	C5-C4	4.25	1.46	1.39
2	Q	401	ATP	C5-C4	4.24	1.46	1.39
2	D	401	ATP	C5-C4	4.24	1.46	1.39
2	K	401	ATP	C5-C4	4.23	1.46	1.39
2	A	401	ATP	C5-C4	4.23	1.46	1.39
2	L	401	ATP	C5-C4	4.22	1.46	1.39
2	T	401	ATP	C5-C4	4.21	1.46	1.39
2	W	401	ATP	C5-C4	4.21	1.46	1.39
2	E	401	ATP	C5-C4	4.20	1.46	1.39
2	M	401	ATP	C5-N7	-2.57	1.34	1.39
2	U	401	ATP	C5-N7	-2.57	1.34	1.39
2	I	401	ATP	C5-N7	-2.56	1.34	1.39
2	N	401	ATP	C5-N7	-2.55	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	401	ATP	C5-N7	-2.55	1.34	1.39
2	C	401	ATP	C5-N7	-2.54	1.34	1.39
2	W	401	ATP	C5-N7	-2.54	1.34	1.39
2	L	401	ATP	C5-N7	-2.54	1.34	1.39
2	V	401	ATP	C5-N7	-2.53	1.34	1.39
2	X	402	ATP	C5-N7	-2.53	1.34	1.39
2	A	401	ATP	C5-N7	-2.53	1.34	1.39
2	D	401	ATP	C5-N7	-2.53	1.34	1.39
2	H	401	ATP	C5-N7	-2.53	1.34	1.39
2	B	401	ATP	C5-N7	-2.53	1.34	1.39
2	J	401	ATP	C5-N7	-2.53	1.34	1.39
2	G	401	ATP	C5-N7	-2.52	1.34	1.39
2	Q	401	ATP	C5-N7	-2.51	1.34	1.39
2	O	401	ATP	C5-N7	-2.51	1.34	1.39
2	P	401	ATP	C5-N7	-2.51	1.34	1.39
2	T	401	ATP	C5-N7	-2.51	1.34	1.39
2	F	401	ATP	C5-N7	-2.50	1.34	1.39
2	K	401	ATP	C5-N7	-2.50	1.34	1.39
2	R	401	ATP	C5-N7	-2.50	1.34	1.39
2	S	401	ATP	C5-N7	-2.50	1.34	1.39
2	E	401	ATP	C5-N7	-2.49	1.34	1.39
2	L	401	ATP	C5-C6	2.41	1.47	1.41
2	W	401	ATP	C5-C6	2.41	1.47	1.41
2	D	401	ATP	C5-C6	2.41	1.47	1.41
2	U	401	ATP	C5-C6	2.40	1.47	1.41
2	C	401	ATP	C5-C6	2.40	1.47	1.41
2	J	401	ATP	C5-C6	2.40	1.47	1.41
2	I	401	ATP	C5-C6	2.40	1.47	1.41
2	T	401	ATP	C5-C6	2.40	1.47	1.41
2	A	401	ATP	C5-C6	2.39	1.47	1.41
2	X	402	ATP	C5-C6	2.39	1.47	1.41
2	N	401	ATP	C5-C6	2.39	1.47	1.41
2	E	401	ATP	C5-C6	2.39	1.47	1.41
2	M	401	ATP	C5-C6	2.39	1.47	1.41
2	V	401	ATP	C5-C6	2.39	1.47	1.41
2	H	401	ATP	C5-C6	2.39	1.47	1.41
2	B	401	ATP	C5-C6	2.39	1.47	1.41
2	S	401	ATP	C5-C6	2.38	1.47	1.41
2	X	401	ATP	C5-C6	2.38	1.47	1.41
2	R	401	ATP	C5-C6	2.38	1.47	1.41
2	G	401	ATP	C5-C6	2.38	1.47	1.41
2	Q	401	ATP	C5-C6	2.37	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	401	ATP	C5-C6	2.37	1.47	1.41
2	F	401	ATP	C5-C6	2.37	1.47	1.41
2	P	401	ATP	C5-C6	2.37	1.47	1.41
2	O	401	ATP	C5-C6	2.36	1.47	1.41
2	M	401	ATP	C8-N7	2.15	1.35	1.31
2	N	401	ATP	C8-N7	2.15	1.35	1.31
2	A	401	ATP	C8-N7	2.14	1.35	1.31
2	C	401	ATP	C8-N7	2.13	1.35	1.31
2	K	401	ATP	C8-N7	2.13	1.35	1.31
2	I	401	ATP	C8-N7	2.13	1.35	1.31
2	X	402	ATP	C8-N7	2.13	1.35	1.31
2	Q	401	ATP	C8-N7	2.12	1.35	1.31
2	J	401	ATP	C8-N7	2.12	1.35	1.31
2	L	401	ATP	C8-N7	2.12	1.35	1.31
2	R	401	ATP	C8-N7	2.11	1.35	1.31
2	G	401	ATP	C8-N7	2.11	1.35	1.31
2	B	401	ATP	C8-N7	2.11	1.35	1.31
2	P	401	ATP	C8-N7	2.11	1.35	1.31
2	X	401	ATP	C8-N7	2.11	1.35	1.31
2	V	401	ATP	C8-N7	2.11	1.35	1.31
2	W	401	ATP	C8-N7	2.10	1.35	1.31
2	E	401	ATP	C8-N7	2.10	1.35	1.31
2	P	401	ATP	C4-N9	-2.10	1.33	1.37
2	G	401	ATP	C4-N9	-2.09	1.33	1.37
2	H	401	ATP	C8-N7	2.09	1.35	1.31
2	T	401	ATP	C8-N7	2.09	1.35	1.31
2	S	401	ATP	C8-N7	2.09	1.35	1.31
2	U	401	ATP	C8-N7	2.09	1.35	1.31
2	X	401	ATP	C4-N9	-2.09	1.33	1.37
2	F	401	ATP	C8-N7	2.09	1.35	1.31
2	R	401	ATP	C4-N9	-2.08	1.33	1.37
2	N	401	ATP	C4-N9	-2.08	1.33	1.37
2	O	401	ATP	C4-N9	-2.08	1.33	1.37
2	D	401	ATP	C8-N7	2.08	1.35	1.31
2	J	401	ATP	C4-N9	-2.08	1.33	1.37
2	Q	401	ATP	C4-N9	-2.07	1.33	1.37
2	A	401	ATP	C4-N9	-2.07	1.33	1.37
2	O	401	ATP	C8-N7	2.07	1.35	1.31
2	F	401	ATP	C4-N9	-2.06	1.33	1.37
2	K	401	ATP	C4-N9	-2.06	1.33	1.37
2	T	401	ATP	C4-N9	-2.06	1.33	1.37
2	L	401	ATP	C4-N9	-2.06	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	ATP	C4-N9	-2.06	1.33	1.37
2	S	401	ATP	C4-N9	-2.05	1.33	1.37
2	W	401	ATP	C4-N9	-2.05	1.33	1.37
2	C	401	ATP	C4-N9	-2.05	1.33	1.37
2	X	402	ATP	C4-N9	-2.05	1.33	1.37
2	H	401	ATP	C4-N9	-2.04	1.33	1.37
2	E	401	ATP	C4-N9	-2.04	1.33	1.37
2	I	401	ATP	C4-N9	-2.04	1.33	1.37
2	V	401	ATP	C4-N9	-2.03	1.33	1.37
2	M	401	ATP	C4-N9	-2.03	1.33	1.37
2	U	401	ATP	C4-N9	-2.02	1.33	1.37
2	D	401	ATP	C4-N9	-2.02	1.33	1.37

All (225) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	401	ATP	C5-C4-N3	-5.73	118.83	126.72
2	R	401	ATP	C5-C4-N3	-5.71	118.86	126.72
2	G	401	ATP	C5-C4-N3	-5.70	118.86	126.72
2	O	401	ATP	C5-C4-N3	-5.69	118.88	126.72
2	X	402	ATP	C5-C4-N3	-5.69	118.89	126.72
2	X	401	ATP	C5-C4-N3	-5.69	118.89	126.72
2	N	401	ATP	C5-C4-N3	-5.68	118.89	126.72
2	Q	401	ATP	C5-C4-N3	-5.68	118.90	126.72
2	K	401	ATP	C5-C4-N3	-5.67	118.90	126.72
2	S	401	ATP	C5-C4-N3	-5.67	118.91	126.72
2	B	401	ATP	C5-C4-N3	-5.67	118.91	126.72
2	T	401	ATP	C5-C4-N3	-5.67	118.91	126.72
2	C	401	ATP	C5-C4-N3	-5.67	118.91	126.72
2	J	401	ATP	C5-C4-N3	-5.67	118.91	126.72
2	H	401	ATP	C5-C4-N3	-5.67	118.92	126.72
2	E	401	ATP	C5-C4-N3	-5.66	118.92	126.72
2	W	401	ATP	C5-C4-N3	-5.66	118.92	126.72
2	F	401	ATP	C5-C4-N3	-5.66	118.93	126.72
2	V	401	ATP	C5-C4-N3	-5.66	118.93	126.72
2	A	401	ATP	C5-C4-N3	-5.66	118.93	126.72
2	U	401	ATP	C5-C4-N3	-5.66	118.93	126.72
2	I	401	ATP	C5-C4-N3	-5.65	118.93	126.72
2	M	401	ATP	C5-C4-N3	-5.65	118.93	126.72
2	L	401	ATP	C5-C4-N3	-5.64	118.94	126.72
2	D	401	ATP	C5-C4-N3	-5.64	118.94	126.72
2	X	402	ATP	N3-C4-N9	4.86	135.44	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	401	ATP	N3-C4-N9	4.86	135.43	127.17
2	P	401	ATP	N3-C4-N9	4.86	135.43	127.17
2	O	401	ATP	N3-C4-N9	4.86	135.43	127.17
2	X	401	ATP	N3-C4-N9	4.85	135.42	127.17
2	I	401	ATP	N3-C4-N9	4.85	135.41	127.17
2	C	401	ATP	N3-C4-N9	4.85	135.41	127.17
2	N	401	ATP	N3-C4-N9	4.84	135.41	127.17
2	D	401	ATP	N3-C4-N9	4.84	135.41	127.17
2	G	401	ATP	N3-C4-N9	4.84	135.40	127.17
2	A	401	ATP	N3-C4-N9	4.84	135.40	127.17
2	J	401	ATP	N3-C4-N9	4.84	135.40	127.17
2	U	401	ATP	N3-C4-N9	4.84	135.40	127.17
2	S	401	ATP	N3-C4-N9	4.84	135.39	127.17
2	H	401	ATP	N3-C4-N9	4.84	135.39	127.17
2	B	401	ATP	N3-C4-N9	4.83	135.39	127.17
2	R	401	ATP	N3-C4-N9	4.83	135.39	127.17
2	T	401	ATP	N3-C4-N9	4.83	135.39	127.17
2	F	401	ATP	N3-C4-N9	4.83	135.37	127.17
2	W	401	ATP	N3-C4-N9	4.82	135.37	127.17
2	K	401	ATP	N3-C4-N9	4.82	135.36	127.17
2	Q	401	ATP	N3-C4-N9	4.82	135.36	127.17
2	V	401	ATP	N3-C4-N9	4.82	135.36	127.17
2	L	401	ATP	N3-C4-N9	4.81	135.35	127.17
2	E	401	ATP	N3-C4-N9	4.81	135.34	127.17
2	X	402	ATP	C2-N3-C4	3.73	120.93	111.83
2	X	401	ATP	C2-N3-C4	3.72	120.92	111.83
2	R	401	ATP	C2-N3-C4	3.72	120.91	111.83
2	P	401	ATP	C2-N3-C4	3.72	120.91	111.83
2	M	401	ATP	C2-N3-C4	3.72	120.91	111.83
2	N	401	ATP	C2-N3-C4	3.72	120.91	111.83
2	S	401	ATP	C2-N3-C4	3.72	120.90	111.83
2	U	401	ATP	C2-N3-C4	3.72	120.90	111.83
2	O	401	ATP	C2-N3-C4	3.71	120.90	111.83
2	D	401	ATP	C2-N3-C4	3.71	120.90	111.83
2	G	401	ATP	C2-N3-C4	3.71	120.90	111.83
2	J	401	ATP	C2-N3-C4	3.71	120.90	111.83
2	I	401	ATP	C2-N3-C4	3.71	120.89	111.83
2	W	401	ATP	C2-N3-C4	3.71	120.89	111.83
2	T	401	ATP	C2-N3-C4	3.71	120.89	111.83
2	K	401	ATP	C2-N3-C4	3.71	120.89	111.83
2	B	401	ATP	C2-N3-C4	3.71	120.89	111.83
2	V	401	ATP	C2-N3-C4	3.71	120.89	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	401	ATP	C2-N3-C4	3.71	120.88	111.83
2	C	401	ATP	C2-N3-C4	3.70	120.87	111.83
2	Q	401	ATP	C2-N3-C4	3.70	120.87	111.83
2	F	401	ATP	C2-N3-C4	3.70	120.86	111.83
2	A	401	ATP	C2-N3-C4	3.69	120.85	111.83
2	E	401	ATP	C2-N3-C4	3.69	120.84	111.83
2	L	401	ATP	C2-N3-C4	3.69	120.84	111.83
2	K	401	ATP	N3-C2-N1	-3.48	123.32	128.58
2	X	401	ATP	N3-C2-N1	-3.47	123.33	128.58
2	J	401	ATP	N3-C2-N1	-3.46	123.34	128.58
2	I	401	ATP	N3-C2-N1	-3.46	123.34	128.58
2	M	401	ATP	N3-C2-N1	-3.46	123.35	128.58
2	D	401	ATP	N3-C2-N1	-3.45	123.35	128.58
2	V	401	ATP	N3-C2-N1	-3.45	123.35	128.58
2	T	401	ATP	N3-C2-N1	-3.45	123.35	128.58
2	W	401	ATP	N3-C2-N1	-3.45	123.36	128.58
2	N	401	ATP	N3-C2-N1	-3.45	123.36	128.58
2	X	402	ATP	N3-C2-N1	-3.45	123.36	128.58
2	U	401	ATP	N3-C2-N1	-3.44	123.37	128.58
2	L	401	ATP	N3-C2-N1	-3.44	123.37	128.58
2	S	401	ATP	N3-C2-N1	-3.44	123.37	128.58
2	B	401	ATP	N3-C2-N1	-3.44	123.37	128.58
2	F	401	ATP	N3-C2-N1	-3.44	123.38	128.58
2	P	401	ATP	N3-C2-N1	-3.44	123.38	128.58
2	Q	401	ATP	N3-C2-N1	-3.43	123.38	128.58
2	G	401	ATP	N3-C2-N1	-3.43	123.39	128.58
2	O	401	ATP	N3-C2-N1	-3.42	123.40	128.58
2	H	401	ATP	N3-C2-N1	-3.42	123.40	128.58
2	R	401	ATP	N3-C2-N1	-3.42	123.40	128.58
2	C	401	ATP	N3-C2-N1	-3.42	123.41	128.58
2	E	401	ATP	N3-C2-N1	-3.41	123.42	128.58
2	A	401	ATP	N3-C2-N1	-3.40	123.43	128.58
2	A	401	ATP	C4-N9-C8	3.38	109.29	105.74
2	M	401	ATP	C4-N9-C8	3.37	109.28	105.74
2	I	401	ATP	C4-N9-C8	3.37	109.28	105.74
2	X	401	ATP	C4-N9-C8	3.37	109.28	105.74
2	J	401	ATP	C4-N9-C8	3.37	109.28	105.74
2	T	401	ATP	C4-N9-C8	3.37	109.27	105.74
2	O	401	ATP	C4-N9-C8	3.36	109.27	105.74
2	X	402	ATP	C4-N9-C8	3.36	109.27	105.74
2	F	401	ATP	C4-N9-C8	3.36	109.27	105.74
2	N	401	ATP	C4-N9-C8	3.36	109.27	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	ATP	C4-N9-C8	3.36	109.26	105.74
2	S	401	ATP	C4-N9-C8	3.35	109.26	105.74
2	G	401	ATP	C4-N9-C8	3.35	109.25	105.74
2	P	401	ATP	C4-N9-C8	3.35	109.25	105.74
2	L	401	ATP	C4-N9-C8	3.34	109.25	105.74
2	B	401	ATP	C4-N9-C8	3.34	109.25	105.74
2	K	401	ATP	C4-N9-C8	3.34	109.24	105.74
2	R	401	ATP	C4-N9-C8	3.34	109.24	105.74
2	H	401	ATP	C4-N9-C8	3.34	109.24	105.74
2	D	401	ATP	C4-N9-C8	3.33	109.24	105.74
2	W	401	ATP	C4-N9-C8	3.33	109.24	105.74
2	V	401	ATP	C4-N9-C8	3.32	109.22	105.74
2	Q	401	ATP	C4-N9-C8	3.31	109.22	105.74
2	E	401	ATP	C4-N9-C8	3.31	109.21	105.74
2	U	401	ATP	C4-N9-C8	3.31	109.21	105.74
2	R	401	ATP	C4-C5-N7	-3.17	106.96	110.58
2	P	401	ATP	C4-C5-N7	-3.15	106.98	110.58
2	G	401	ATP	C4-C5-N7	-3.15	106.98	110.58
2	O	401	ATP	C4-C5-N7	-3.15	106.98	110.58
2	S	401	ATP	C4-C5-N7	-3.15	106.98	110.58
2	F	401	ATP	C4-C5-N7	-3.14	107.00	110.58
2	E	401	ATP	C4-C5-N7	-3.13	107.00	110.58
2	K	401	ATP	C4-C5-N7	-3.13	107.00	110.58
2	X	401	ATP	C4-C5-N7	-3.13	107.00	110.58
2	T	401	ATP	C4-C5-N7	-3.13	107.01	110.58
2	V	401	ATP	C4-C5-N7	-3.12	107.01	110.58
2	Q	401	ATP	C4-C5-N7	-3.12	107.01	110.58
2	B	401	ATP	C4-C5-N7	-3.12	107.02	110.58
2	H	401	ATP	C4-C5-N7	-3.12	107.02	110.58
2	L	401	ATP	C4-C5-N7	-3.11	107.03	110.58
2	I	401	ATP	C4-C5-N7	-3.11	107.03	110.58
2	N	401	ATP	C4-C5-N7	-3.10	107.04	110.58
2	J	401	ATP	C4-C5-N7	-3.10	107.04	110.58
2	C	401	ATP	C4-C5-N7	-3.10	107.04	110.58
2	U	401	ATP	C4-C5-N7	-3.09	107.04	110.58
2	W	401	ATP	C4-C5-N7	-3.09	107.05	110.58
2	X	402	ATP	C4-C5-N7	-3.09	107.05	110.58
2	D	401	ATP	C4-C5-N7	-3.08	107.06	110.58
2	A	401	ATP	C4-C5-N7	-3.07	107.07	110.58
2	M	401	ATP	C4-C5-N7	-3.07	107.07	110.58
2	V	401	ATP	C5-N7-C8	2.58	107.50	103.45
2	O	401	ATP	C5-N7-C8	2.58	107.50	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	401	ATP	C5-N7-C8	2.58	107.50	103.45
2	F	401	ATP	C5-N7-C8	2.57	107.49	103.45
2	G	401	ATP	C5-N7-C8	2.57	107.48	103.45
2	U	401	ATP	C5-N7-C8	2.56	107.48	103.45
2	I	401	ATP	C5-N7-C8	2.56	107.48	103.45
2	T	401	ATP	C5-N7-C8	2.56	107.48	103.45
2	H	401	ATP	C5-N7-C8	2.56	107.48	103.45
2	L	401	ATP	C5-N7-C8	2.56	107.48	103.45
2	P	401	ATP	C5-N7-C8	2.56	107.48	103.45
2	M	401	ATP	C5-N7-C8	2.56	107.48	103.45
2	R	401	ATP	C5-N7-C8	2.56	107.48	103.45
2	B	401	ATP	C5-N7-C8	2.55	107.46	103.45
2	W	401	ATP	C5-N7-C8	2.55	107.46	103.45
2	X	401	ATP	C5-N7-C8	2.55	107.46	103.45
2	X	402	ATP	C5-N7-C8	2.55	107.46	103.45
2	N	401	ATP	C5-N7-C8	2.55	107.45	103.45
2	C	401	ATP	C5-N7-C8	2.54	107.45	103.45
2	J	401	ATP	C5-N7-C8	2.54	107.44	103.45
2	D	401	ATP	C5-N7-C8	2.54	107.44	103.45
2	Q	401	ATP	C5-N7-C8	2.54	107.44	103.45
2	E	401	ATP	C5-N7-C8	2.53	107.43	103.45
2	K	401	ATP	C5-N7-C8	2.53	107.43	103.45
2	A	401	ATP	C5-N7-C8	2.53	107.43	103.45
2	M	401	ATP	N9-C8-N7	-2.39	110.55	113.94
2	L	401	ATP	N9-C8-N7	-2.39	110.55	113.94
2	T	401	ATP	N9-C8-N7	-2.38	110.55	113.94
2	N	401	ATP	N9-C8-N7	-2.38	110.56	113.94
2	A	401	ATP	N9-C8-N7	-2.38	110.56	113.94
2	X	402	ATP	N9-C8-N7	-2.38	110.56	113.94
2	V	401	ATP	N9-C8-N7	-2.38	110.56	113.94
2	P	401	ATP	N9-C8-N7	-2.38	110.56	113.94
2	F	401	ATP	N9-C8-N7	-2.38	110.56	113.94
2	G	401	ATP	N9-C8-N7	-2.38	110.57	113.94
2	W	401	ATP	N9-C8-N7	-2.37	110.57	113.94
2	I	401	ATP	N9-C8-N7	-2.37	110.57	113.94
2	O	401	ATP	N9-C8-N7	-2.37	110.57	113.94
2	J	401	ATP	N9-C8-N7	-2.37	110.57	113.94
2	R	401	ATP	N9-C8-N7	-2.37	110.58	113.94
2	S	401	ATP	N9-C8-N7	-2.36	110.58	113.94
2	B	401	ATP	N9-C8-N7	-2.36	110.58	113.94
2	C	401	ATP	N9-C8-N7	-2.36	110.58	113.94
2	X	401	ATP	N9-C8-N7	-2.36	110.58	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	401	ATP	N9-C8-N7	-2.36	110.59	113.94
2	Q	401	ATP	N9-C8-N7	-2.35	110.60	113.94
2	U	401	ATP	N9-C8-N7	-2.35	110.60	113.94
2	K	401	ATP	N9-C8-N7	-2.35	110.61	113.94
2	D	401	ATP	N9-C8-N7	-2.33	110.63	113.94
2	E	401	ATP	N9-C8-N7	-2.33	110.63	113.94
2	V	401	ATP	N6-C6-N1	2.15	123.16	118.38
2	S	401	ATP	N6-C6-N1	2.15	123.16	118.38
2	L	401	ATP	N6-C6-N1	2.15	123.16	118.38
2	E	401	ATP	N6-C6-N1	2.14	123.15	118.38
2	U	401	ATP	N6-C6-N1	2.14	123.15	118.38
2	T	401	ATP	N6-C6-N1	2.14	123.14	118.38
2	J	401	ATP	N6-C6-N1	2.14	123.14	118.38
2	G	401	ATP	N6-C6-N1	2.14	123.13	118.38
2	X	402	ATP	N6-C6-N1	2.14	123.13	118.38
2	P	401	ATP	N6-C6-N1	2.14	123.13	118.38
2	H	401	ATP	N6-C6-N1	2.13	123.13	118.38
2	R	401	ATP	N6-C6-N1	2.13	123.13	118.38
2	D	401	ATP	N6-C6-N1	2.13	123.13	118.38
2	K	401	ATP	N6-C6-N1	2.13	123.13	118.38
2	I	401	ATP	N6-C6-N1	2.13	123.13	118.38
2	B	401	ATP	N6-C6-N1	2.13	123.12	118.38
2	W	401	ATP	N6-C6-N1	2.13	123.12	118.38
2	Q	401	ATP	N6-C6-N1	2.13	123.11	118.38
2	M	401	ATP	N6-C6-N1	2.13	123.11	118.38
2	F	401	ATP	N6-C6-N1	2.12	123.11	118.38
2	X	401	ATP	N6-C6-N1	2.12	123.11	118.38
2	N	401	ATP	N6-C6-N1	2.12	123.09	118.38
2	A	401	ATP	N6-C6-N1	2.12	123.09	118.38
2	C	401	ATP	N6-C6-N1	2.11	123.08	118.38
2	O	401	ATP	N6-C6-N1	2.11	123.08	118.38

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	ATP	PA-O3A-PB-O2B
2	B	401	ATP	PA-O3A-PB-O2B
2	C	401	ATP	PA-O3A-PB-O2B
2	D	401	ATP	PA-O3A-PB-O2B
2	E	401	ATP	PA-O3A-PB-O2B
2	F	401	ATP	PA-O3A-PB-O2B

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Mol	Chain	Res	Type	Atoms
2	G	401	ATP	PA-O3A-PB-O2B
2	H	401	ATP	PA-O3A-PB-O2B
2	I	401	ATP	PA-O3A-PB-O2B
2	J	401	ATP	PA-O3A-PB-O2B
2	K	401	ATP	PA-O3A-PB-O2B
2	L	401	ATP	PA-O3A-PB-O2B
2	M	401	ATP	PA-O3A-PB-O2B
2	N	401	ATP	PA-O3A-PB-O2B
2	O	401	ATP	PA-O3A-PB-O2B
2	P	401	ATP	PA-O3A-PB-O2B
2	Q	401	ATP	PA-O3A-PB-O2B
2	R	401	ATP	PA-O3A-PB-O2B
2	S	401	ATP	PA-O3A-PB-O2B
2	T	401	ATP	PA-O3A-PB-O2B
2	U	401	ATP	PA-O3A-PB-O2B
2	V	401	ATP	PA-O3A-PB-O2B
2	W	401	ATP	PA-O3A-PB-O2B
2	X	401	ATP	PA-O3A-PB-O2B
2	X	402	ATP	PA-O3A-PB-O2B

There are no ring outliers.

25 monomers are involved in 105 short contacts:

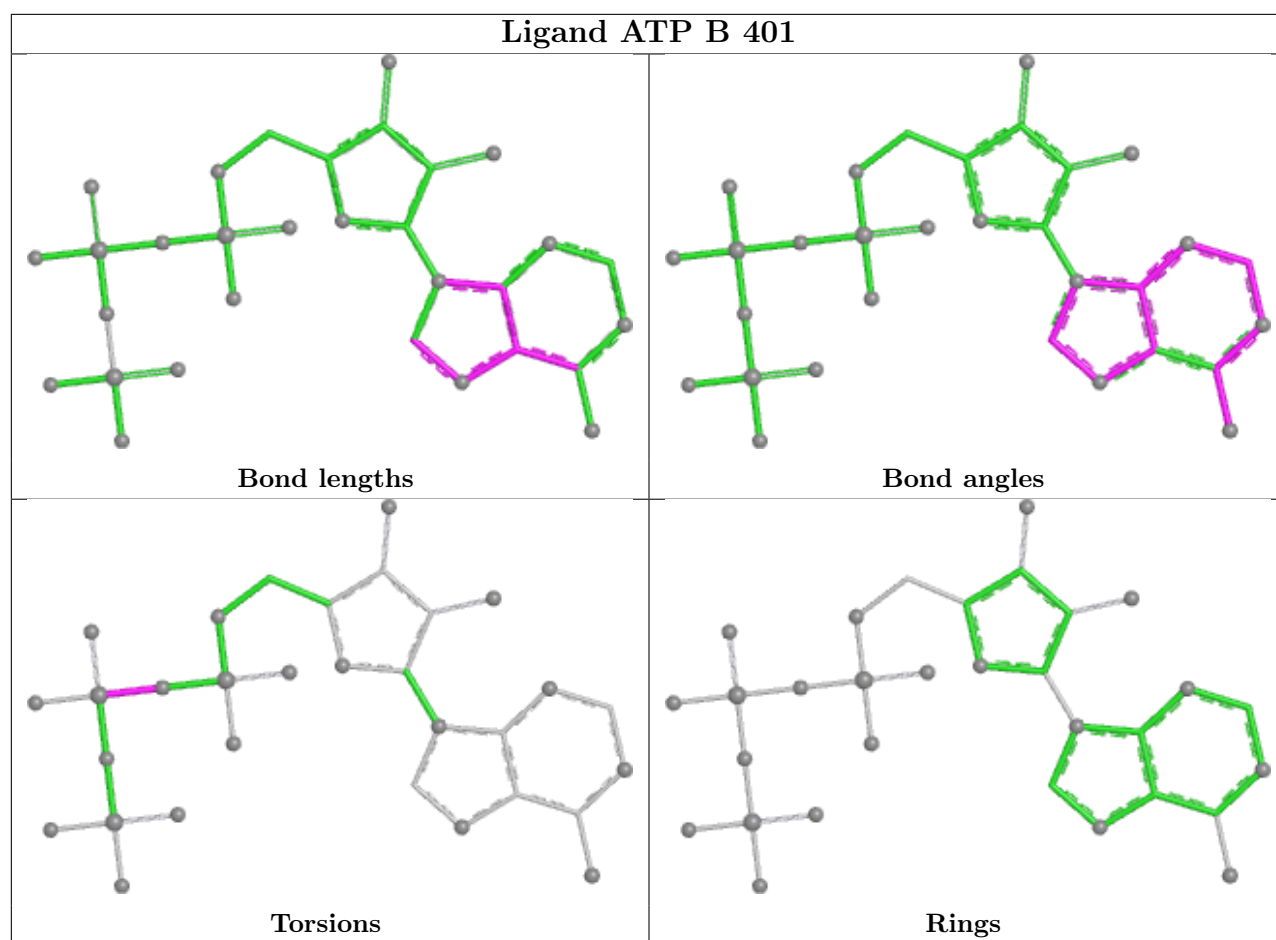
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	ATP	5	0
2	J	401	ATP	4	0
2	H	401	ATP	4	0
2	G	401	ATP	4	0
2	X	401	ATP	4	0
2	A	401	ATP	4	0
2	S	401	ATP	4	0
2	Q	401	ATP	5	0
2	N	401	ATP	4	0
2	X	402	ATP	1	0
2	T	401	ATP	5	0
2	F	401	ATP	4	0
2	K	401	ATP	4	0
2	V	401	ATP	4	0
2	I	401	ATP	4	0
2	L	401	ATP	4	0
2	E	401	ATP	4	0
2	U	401	ATP	5	0

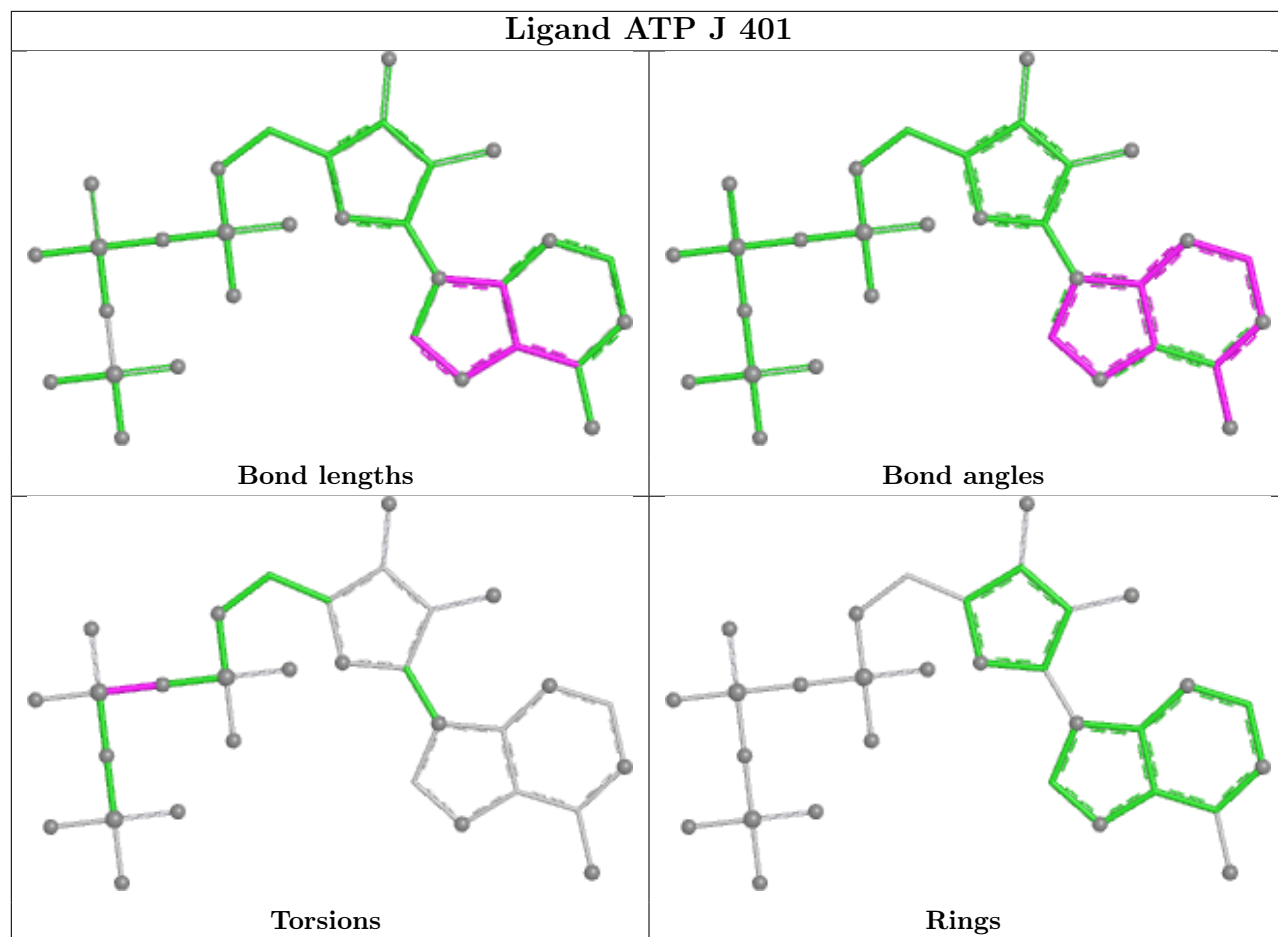
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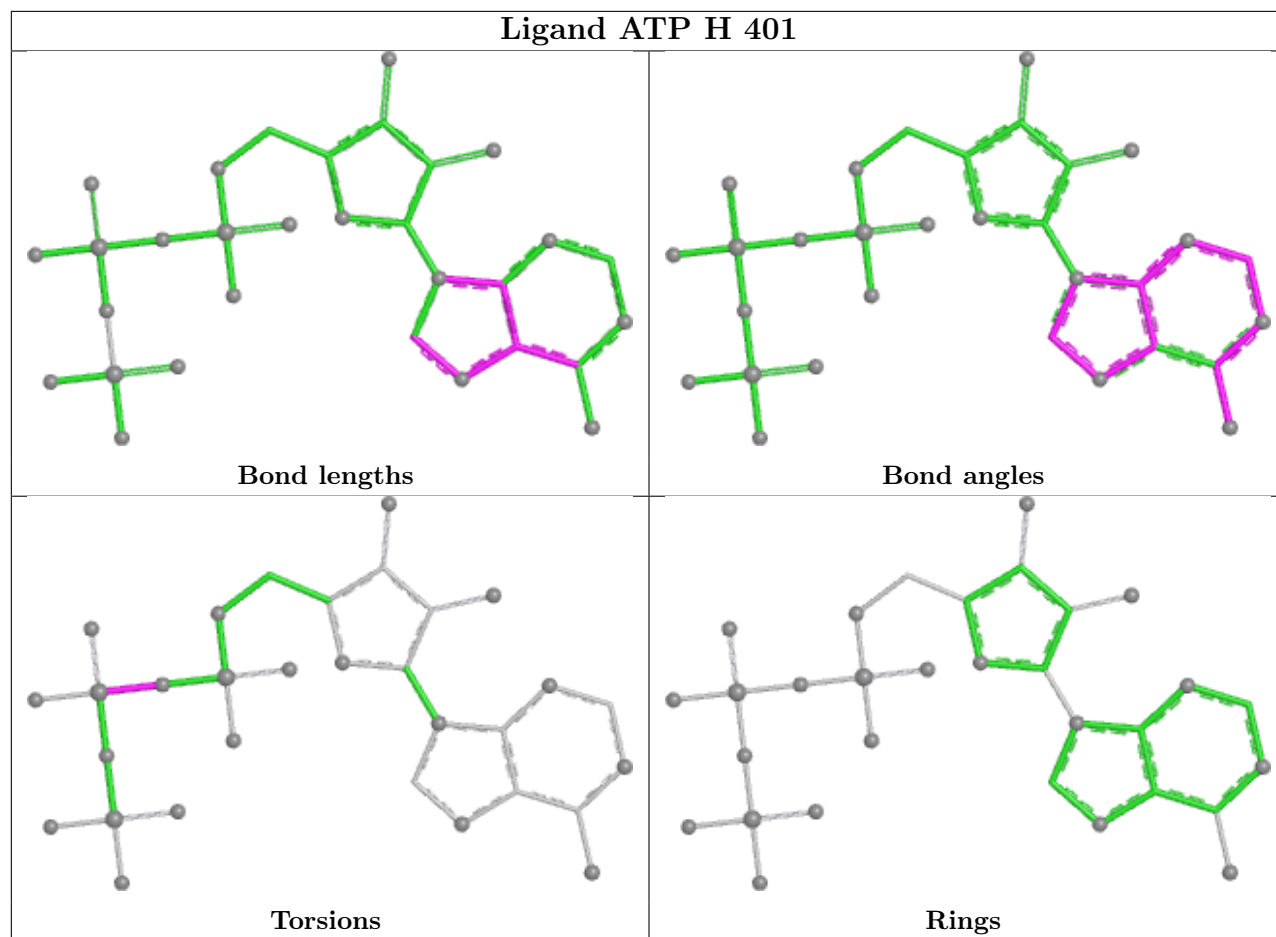
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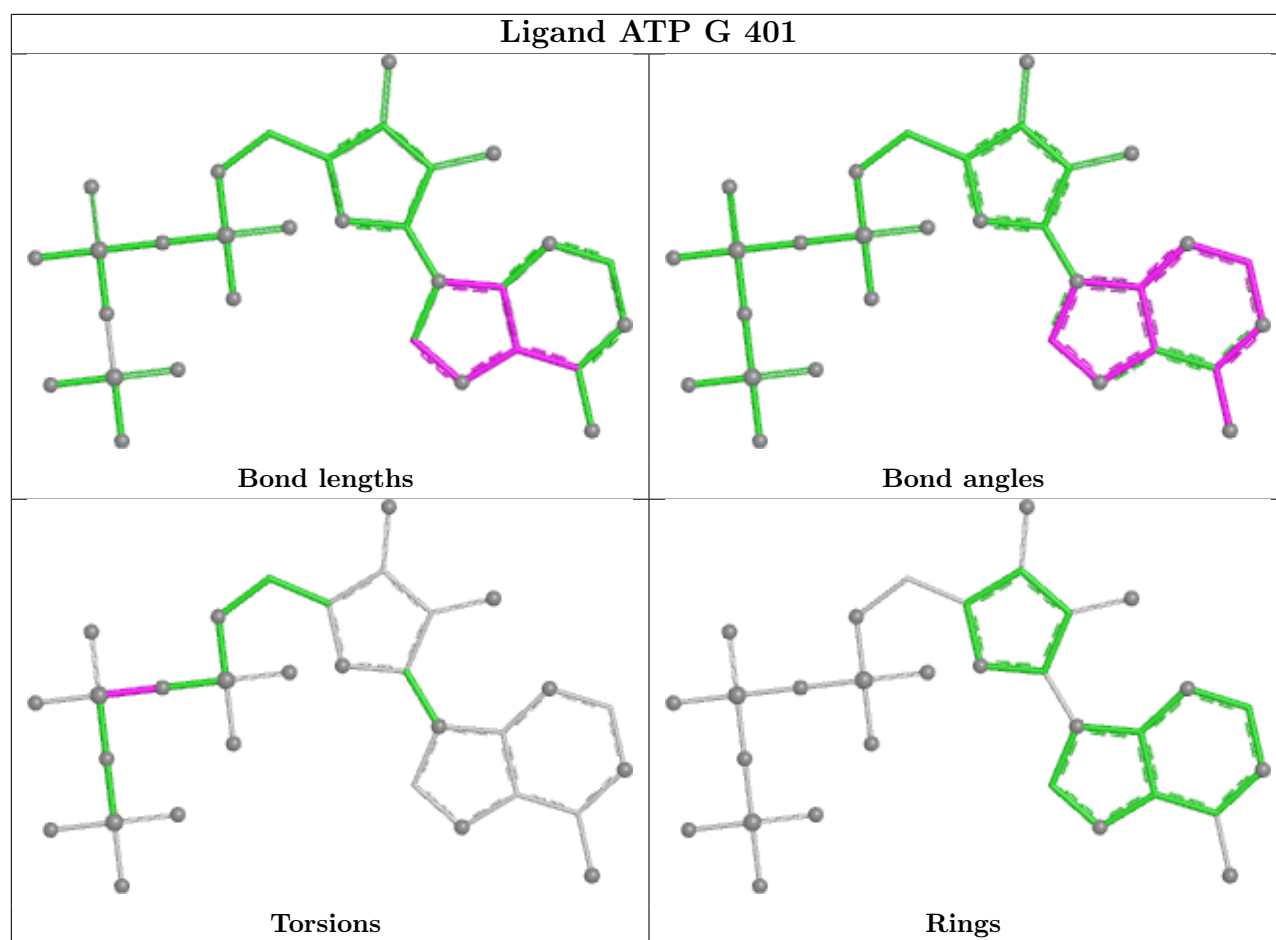
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	ATP	4	0
2	W	401	ATP	4	0
2	M	401	ATP	4	0
2	R	401	ATP	5	0
2	P	401	ATP	5	0
2	O	401	ATP	5	0
2	C	401	ATP	5	0

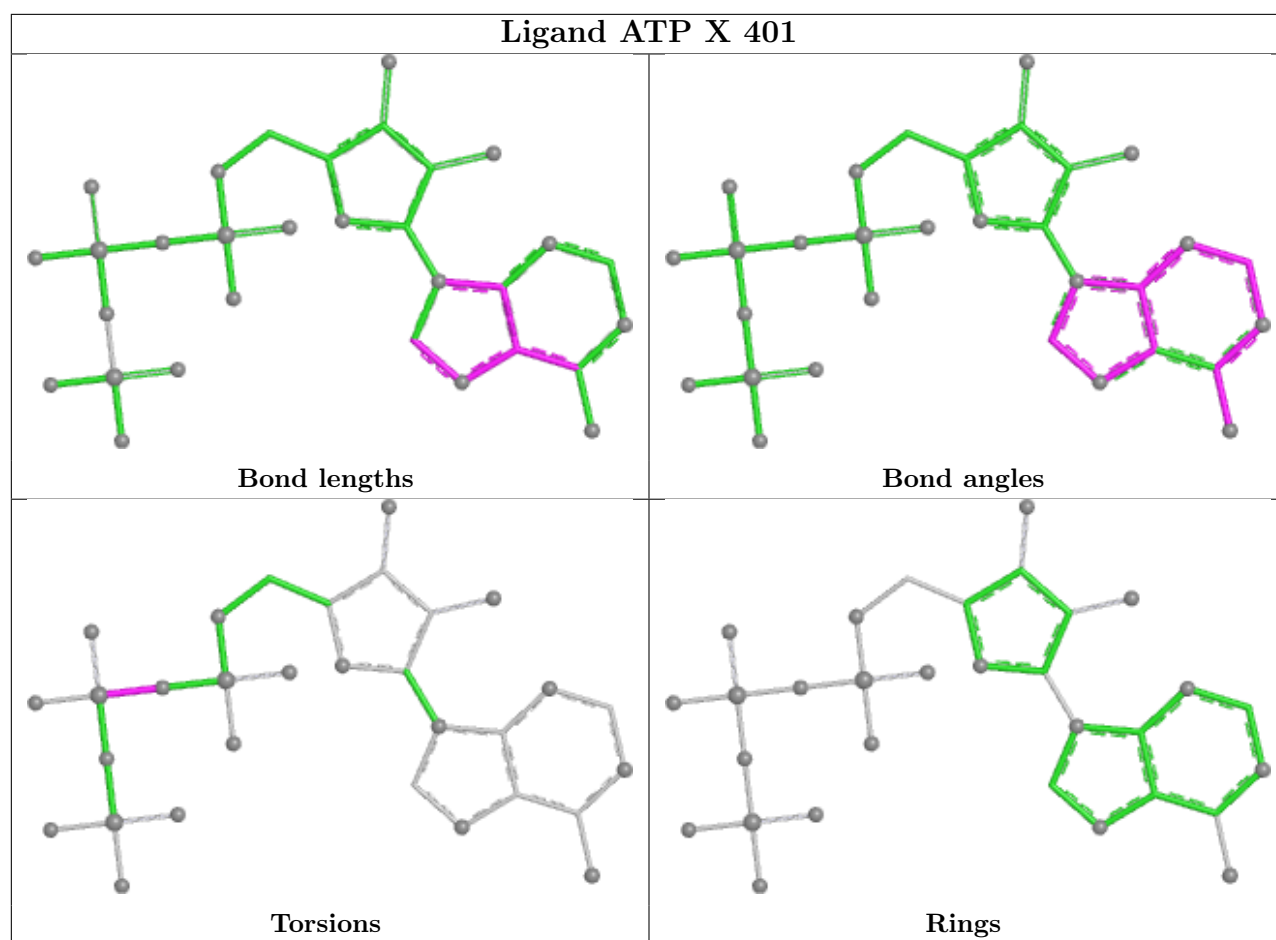
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

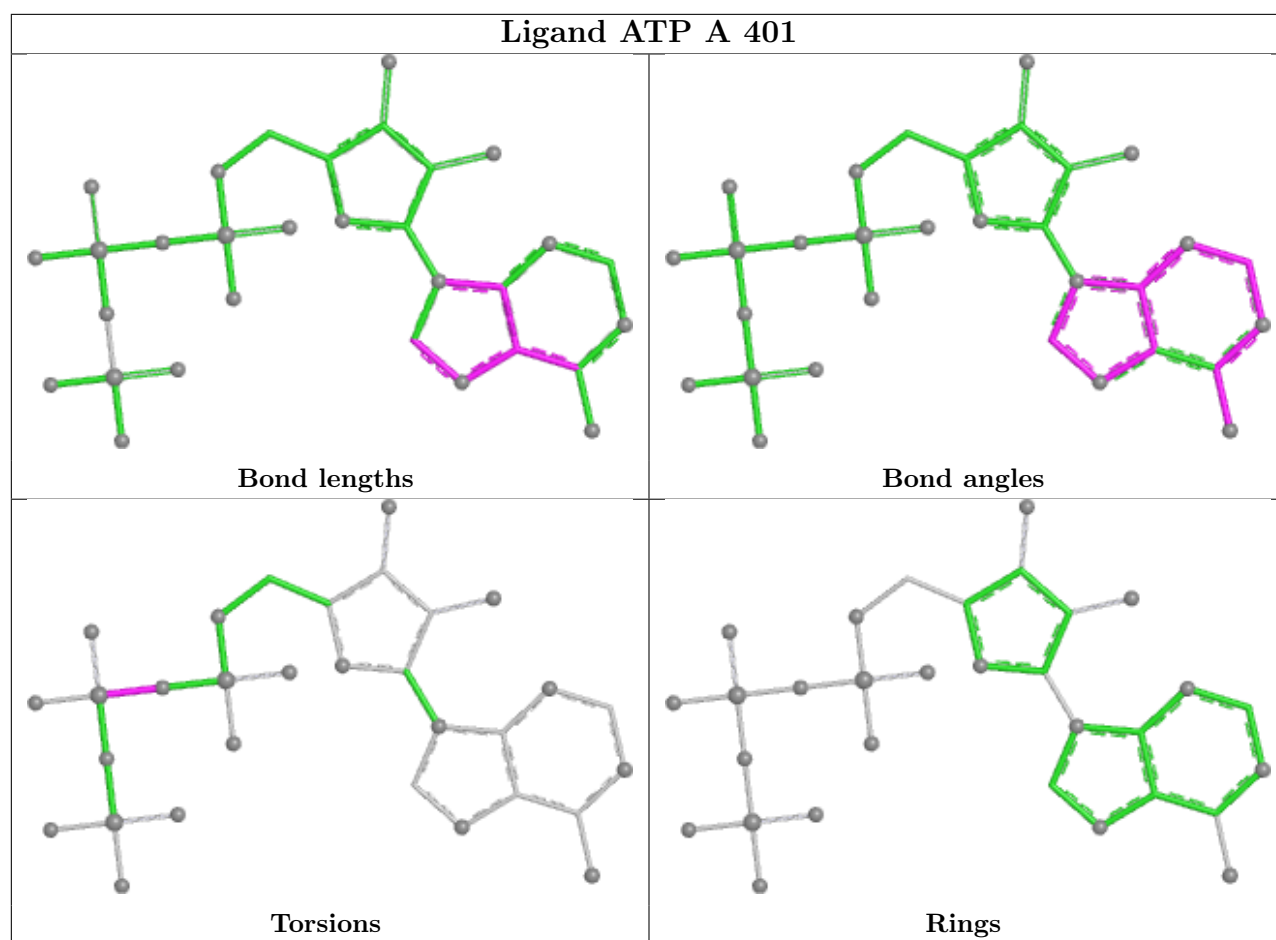


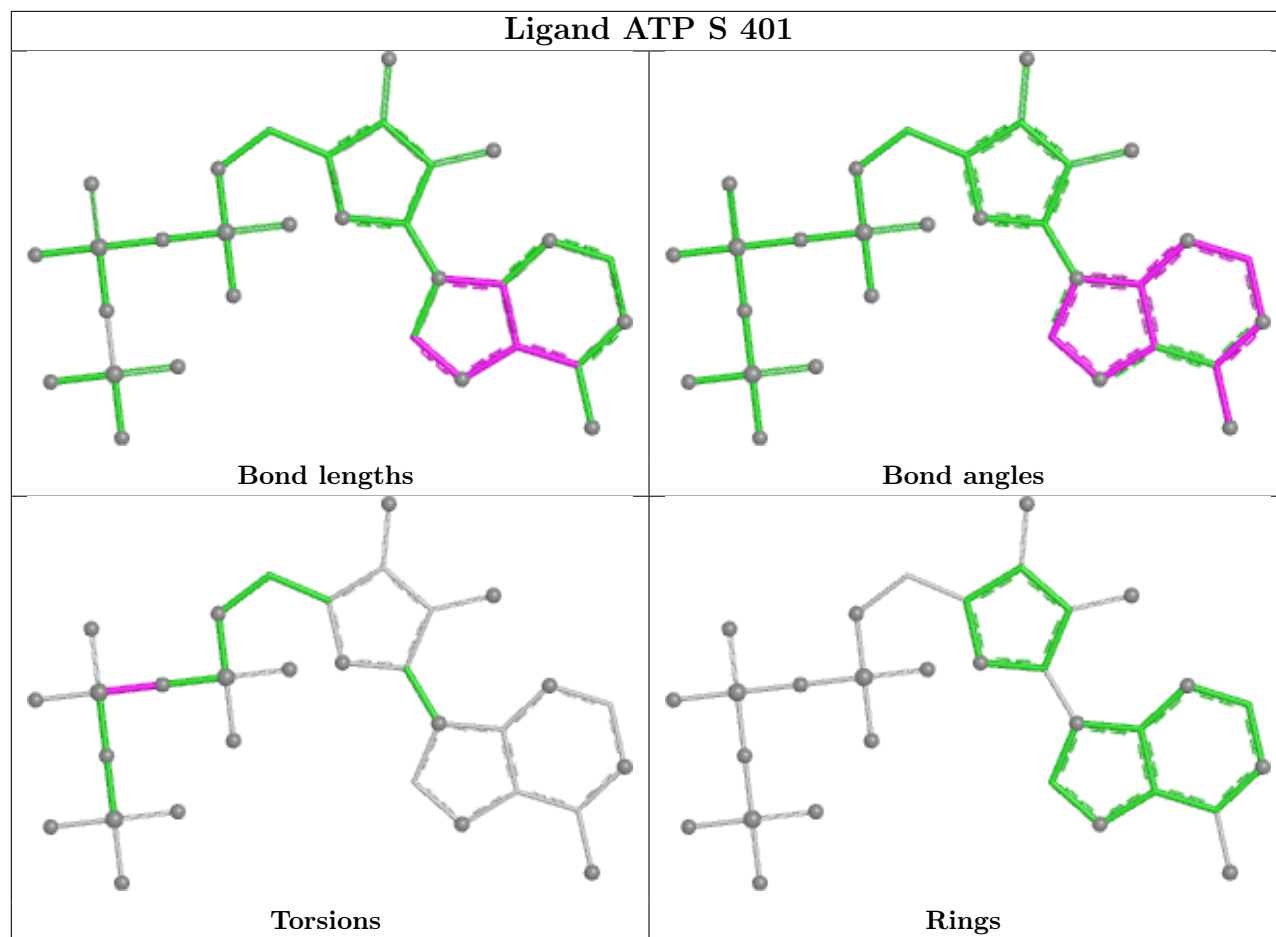


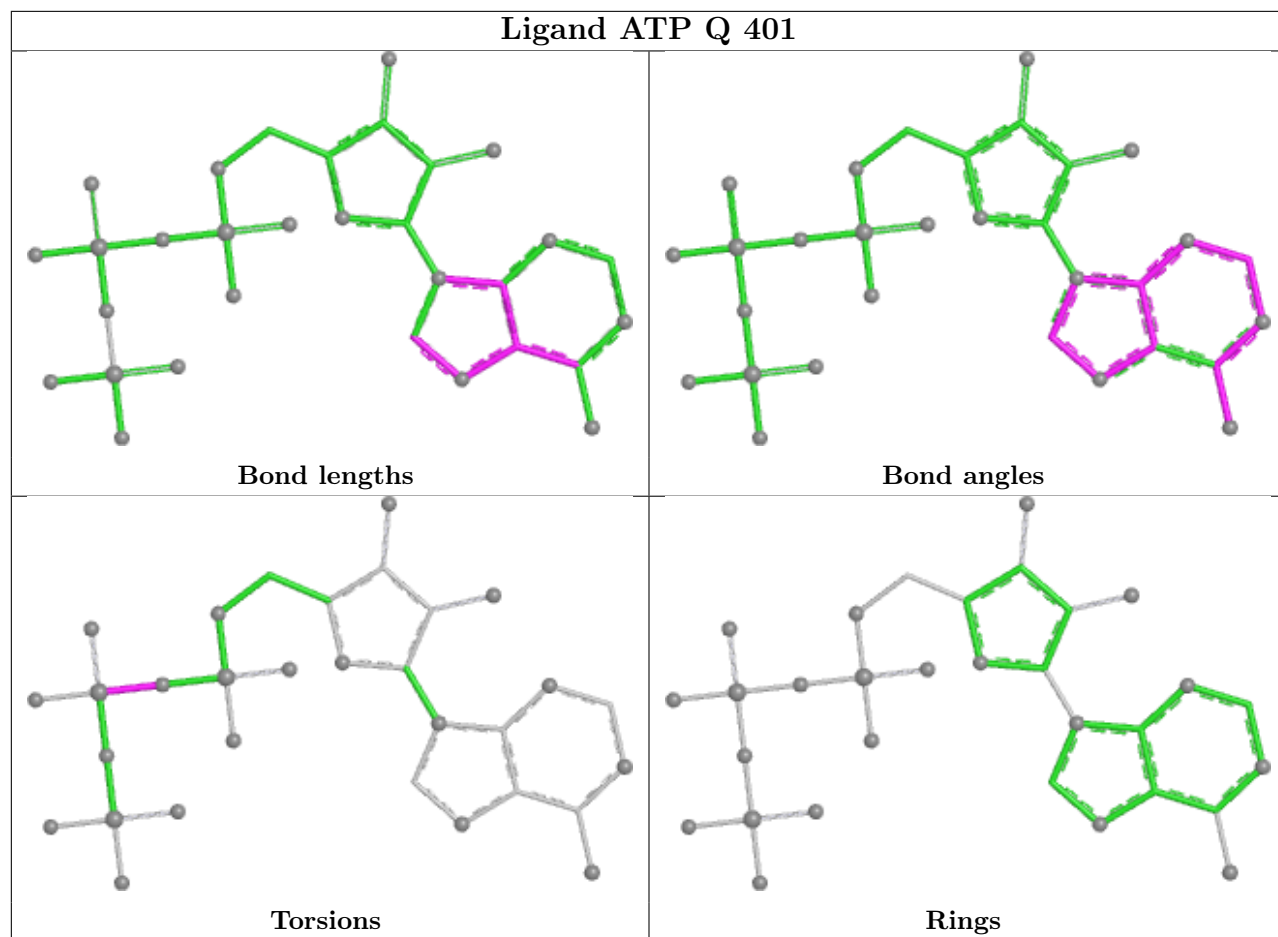


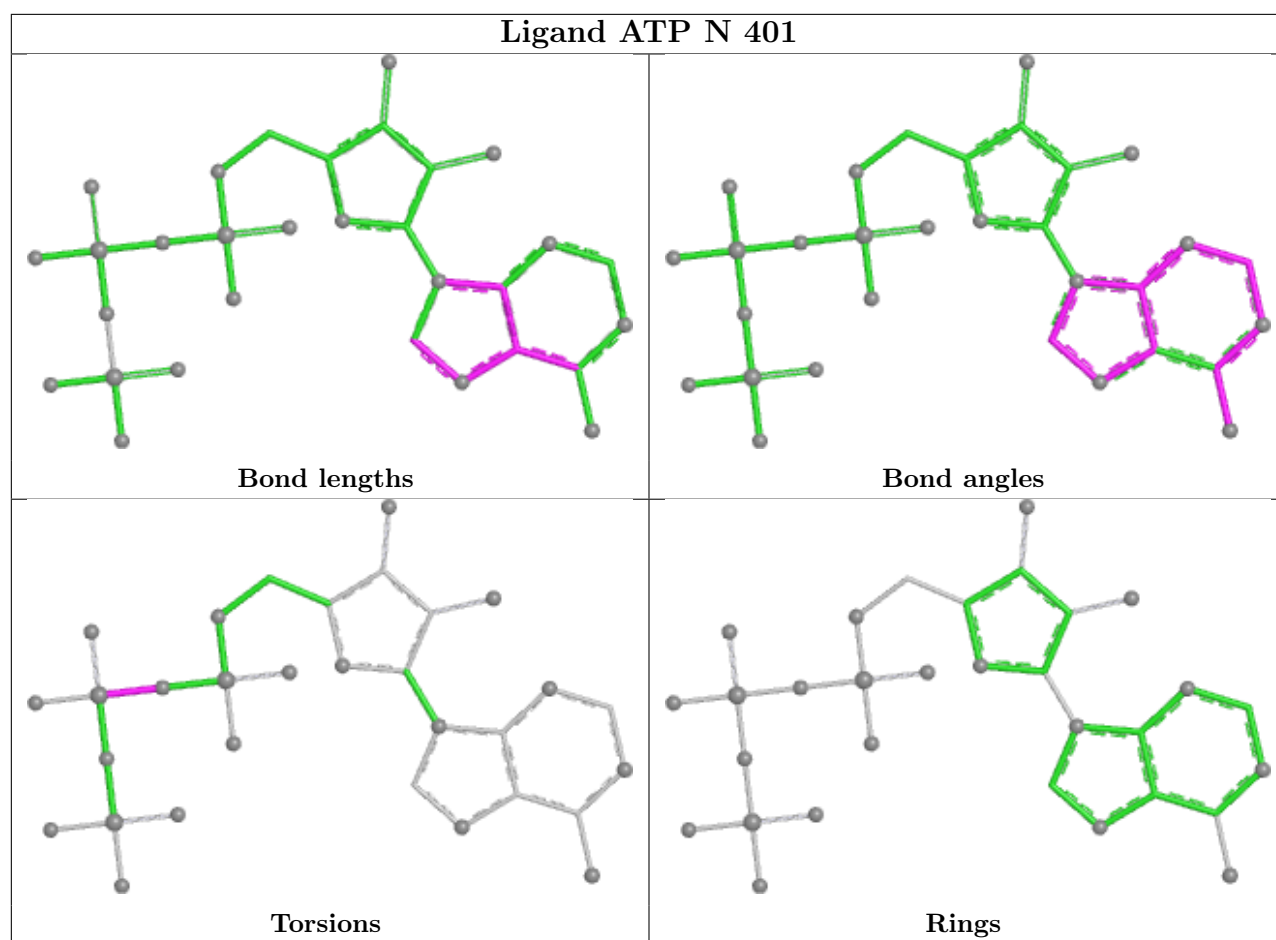


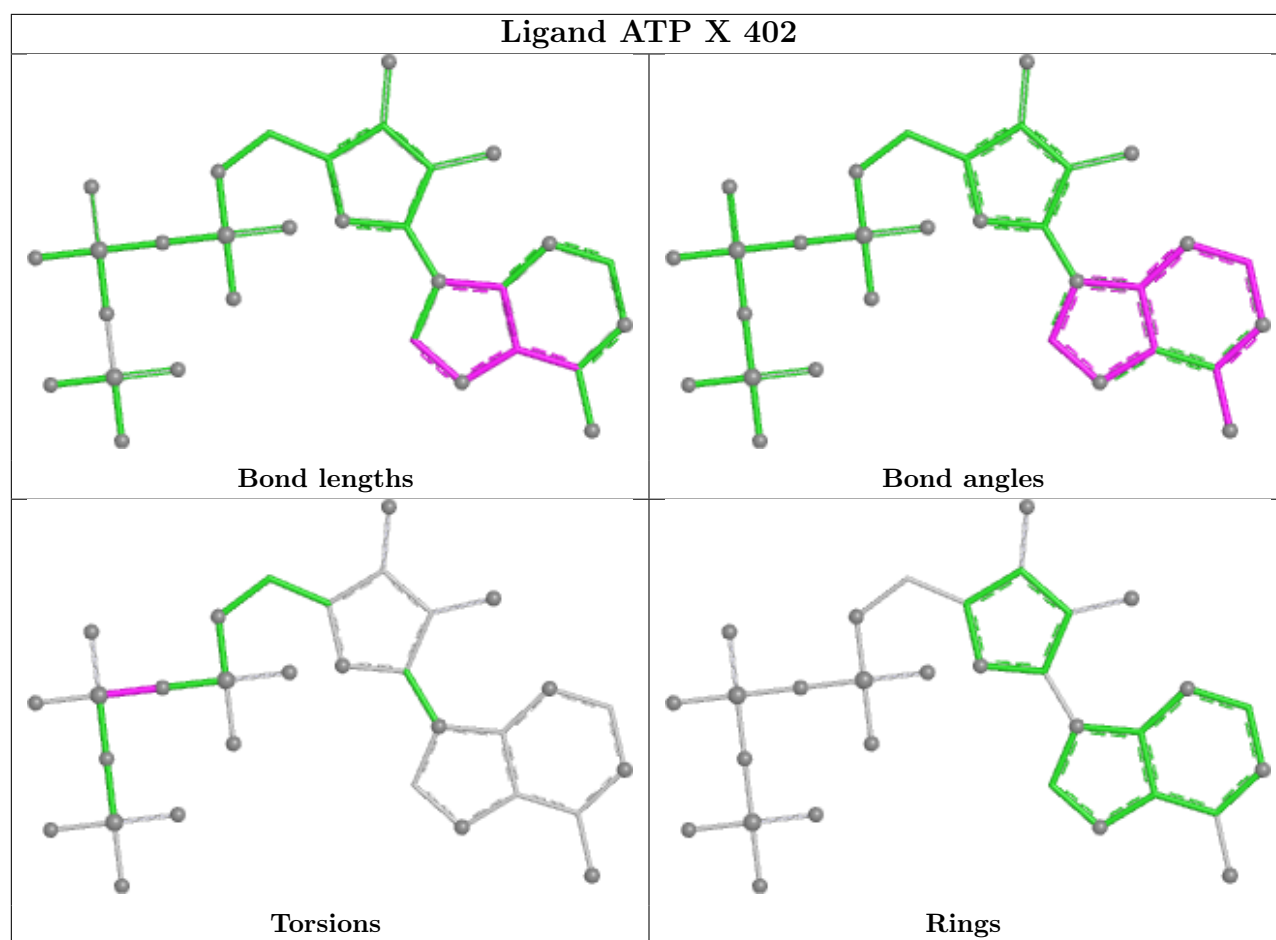


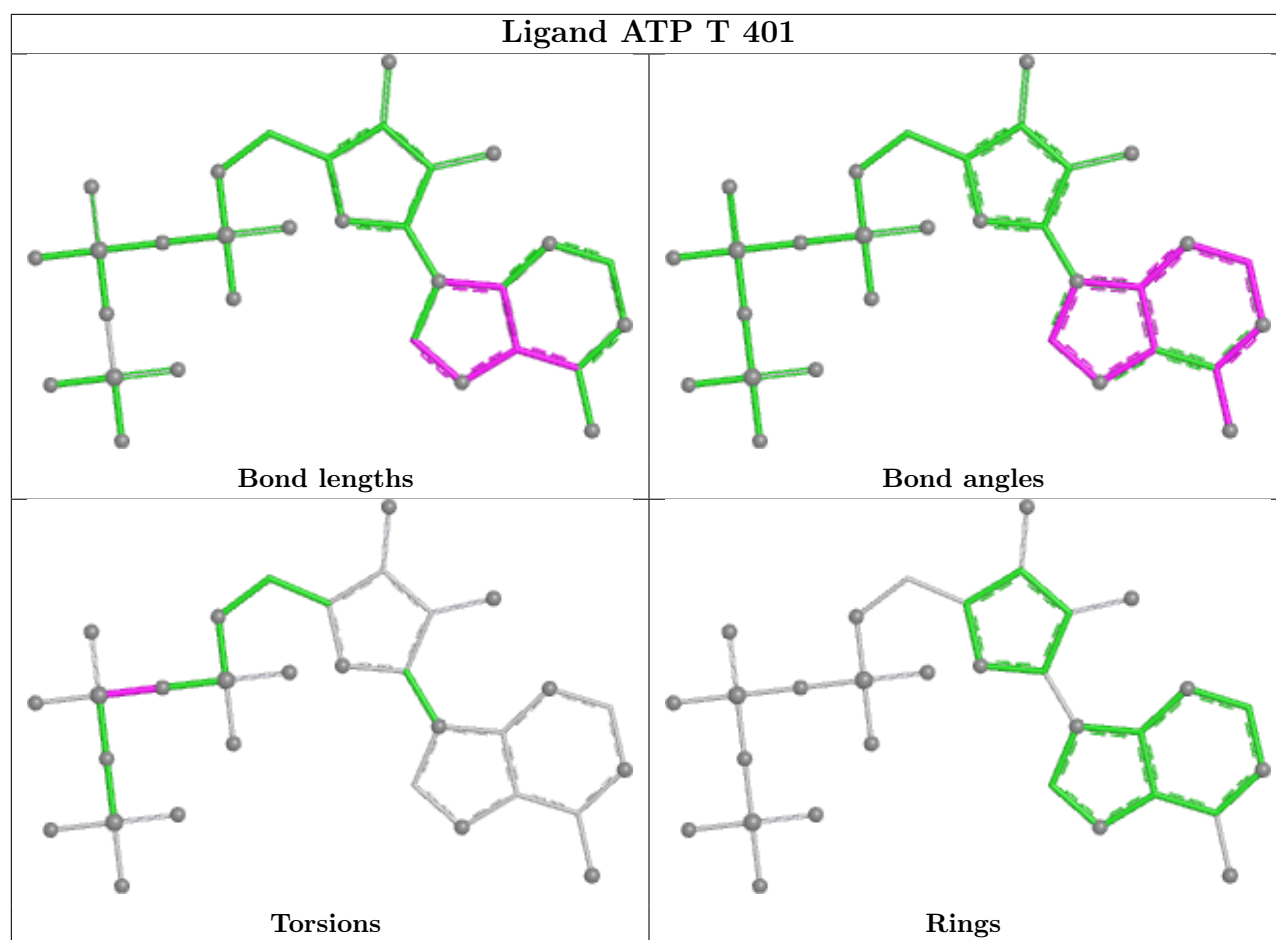


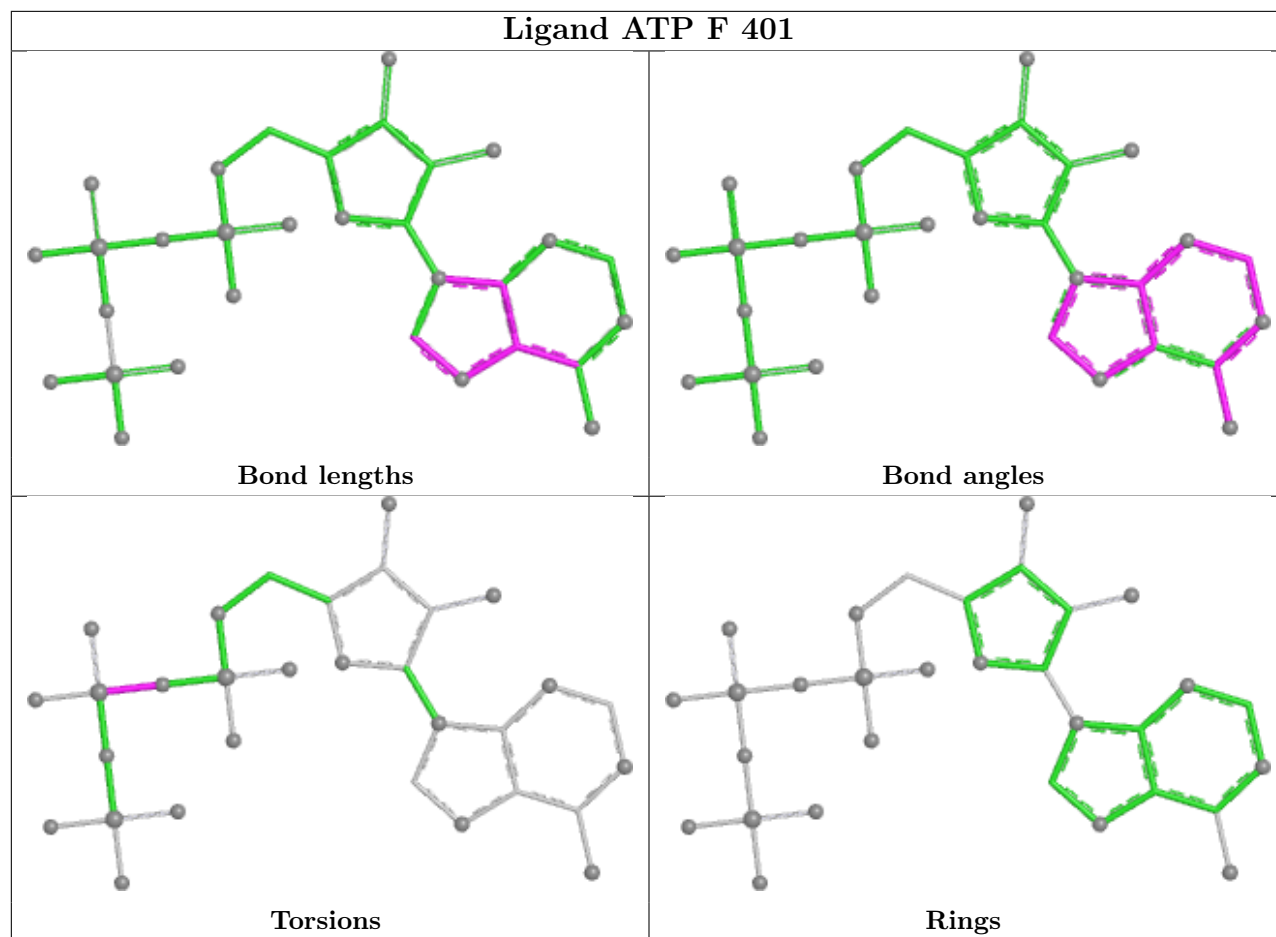


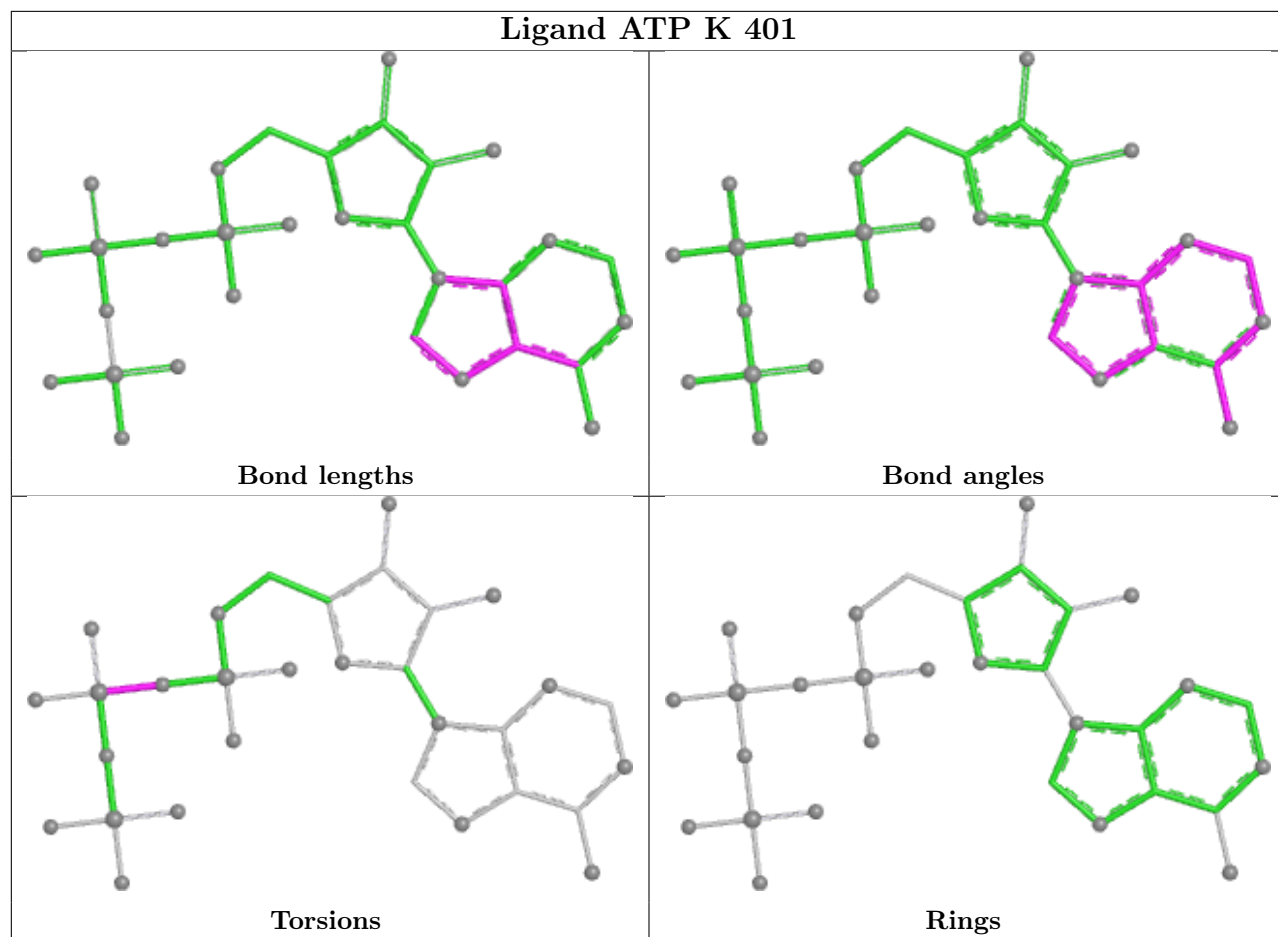


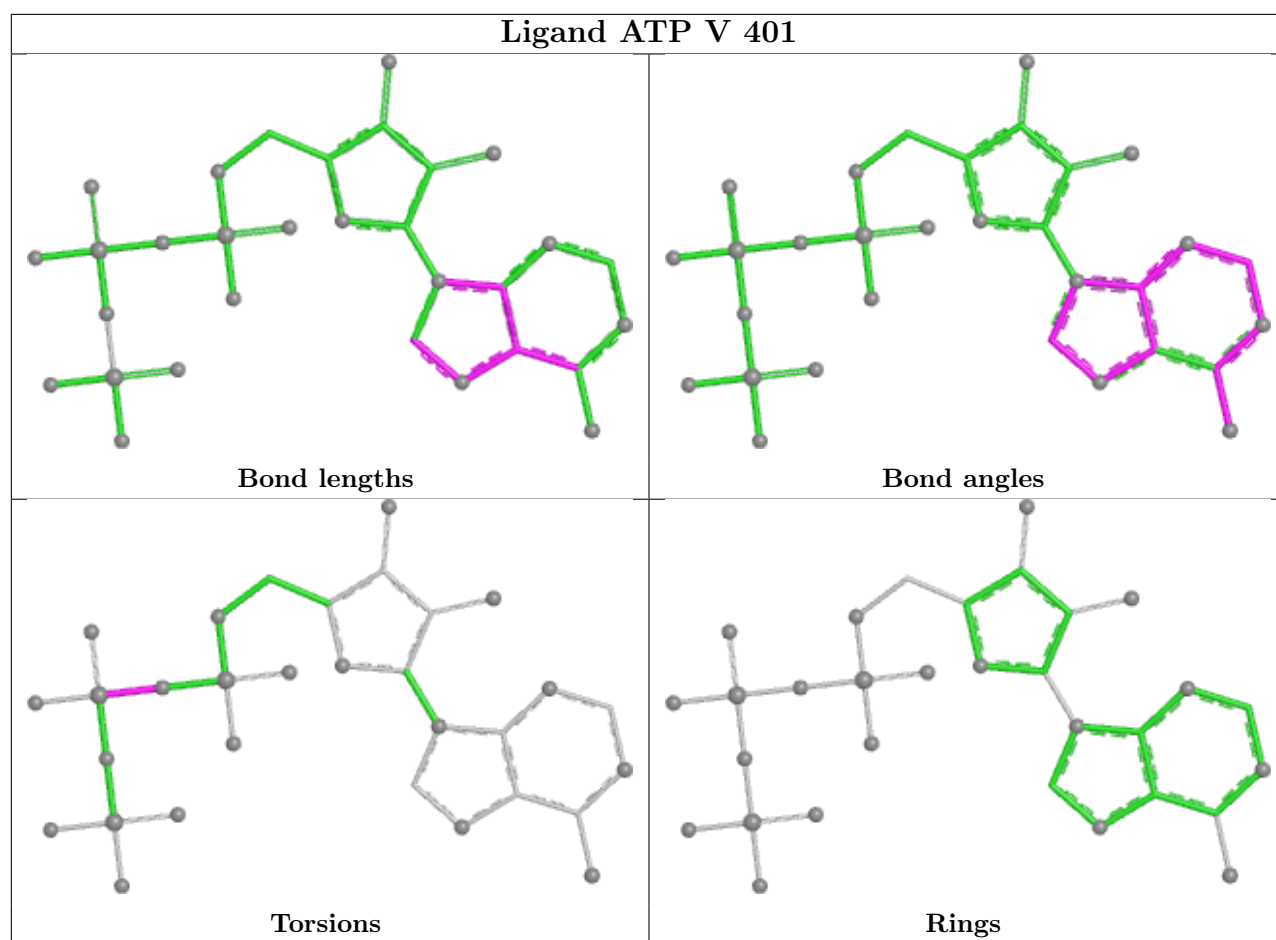


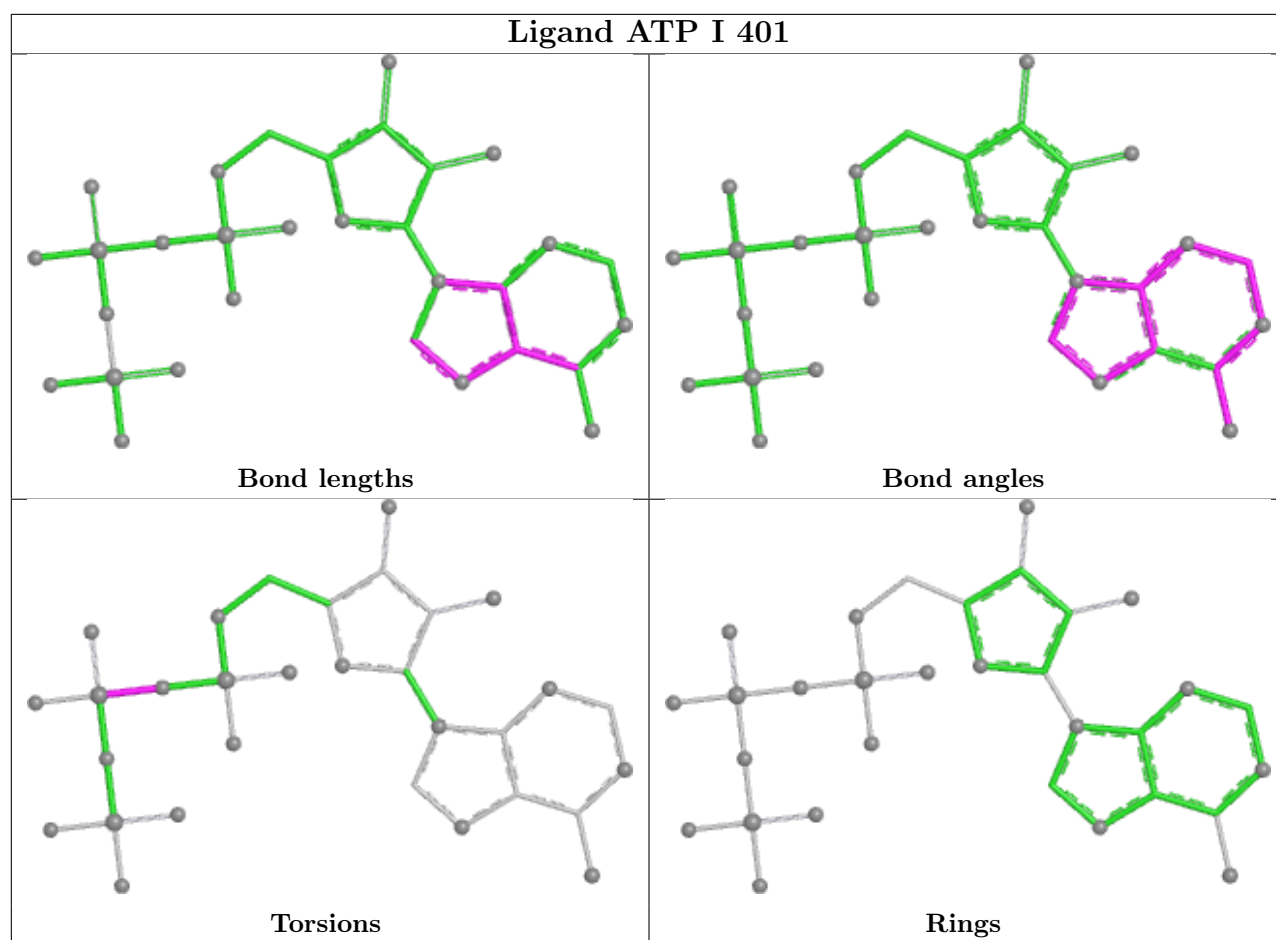


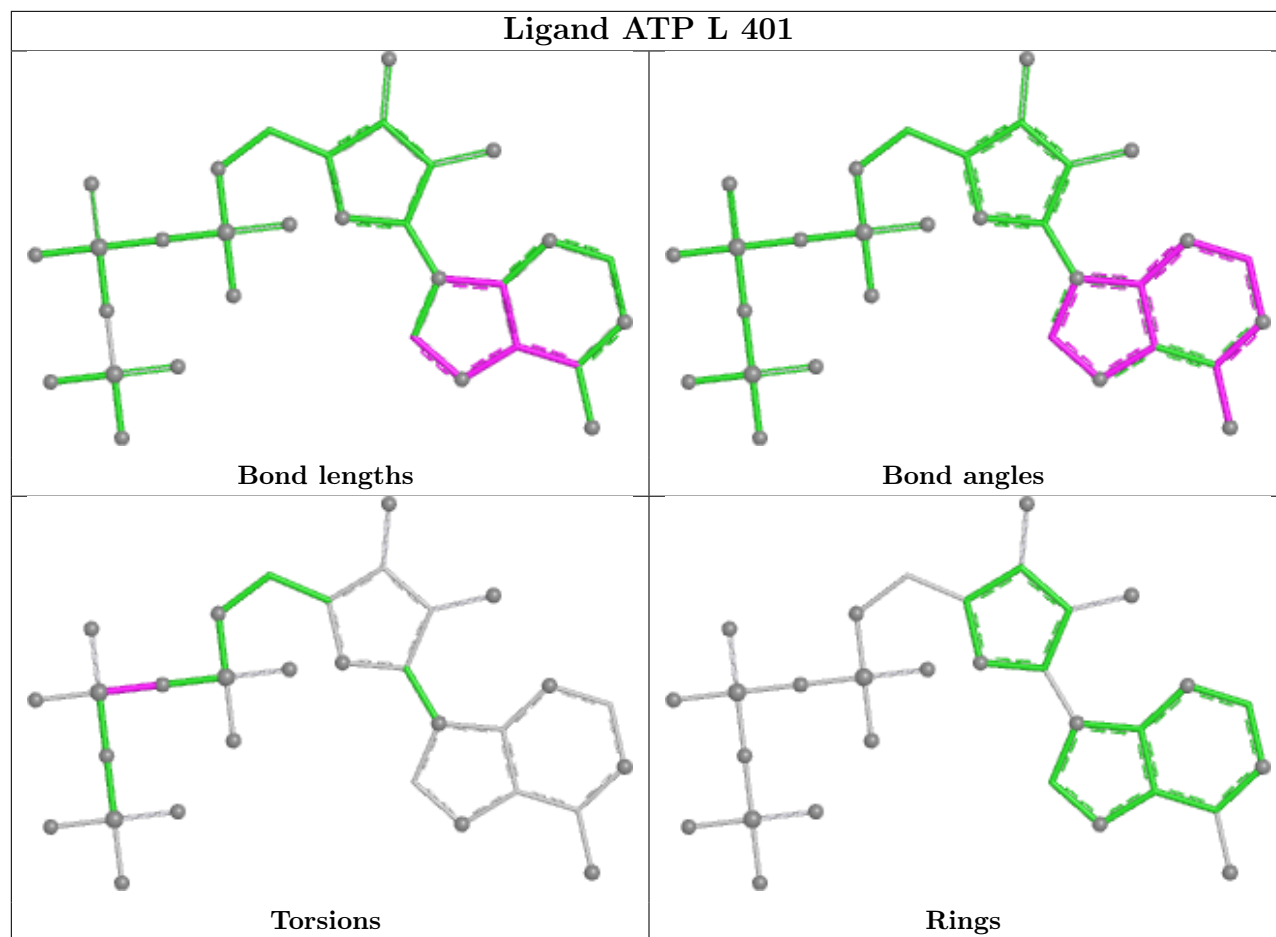


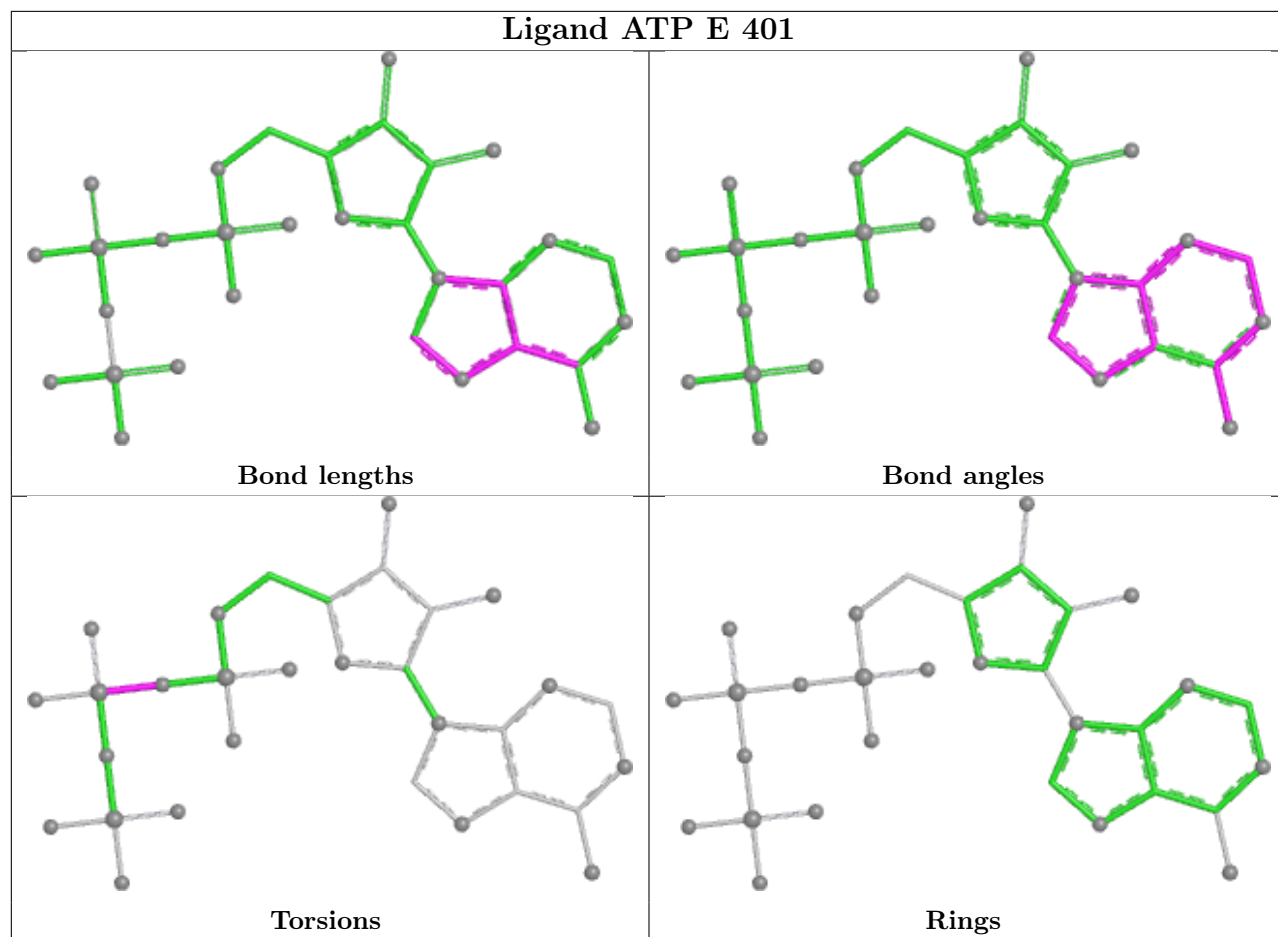


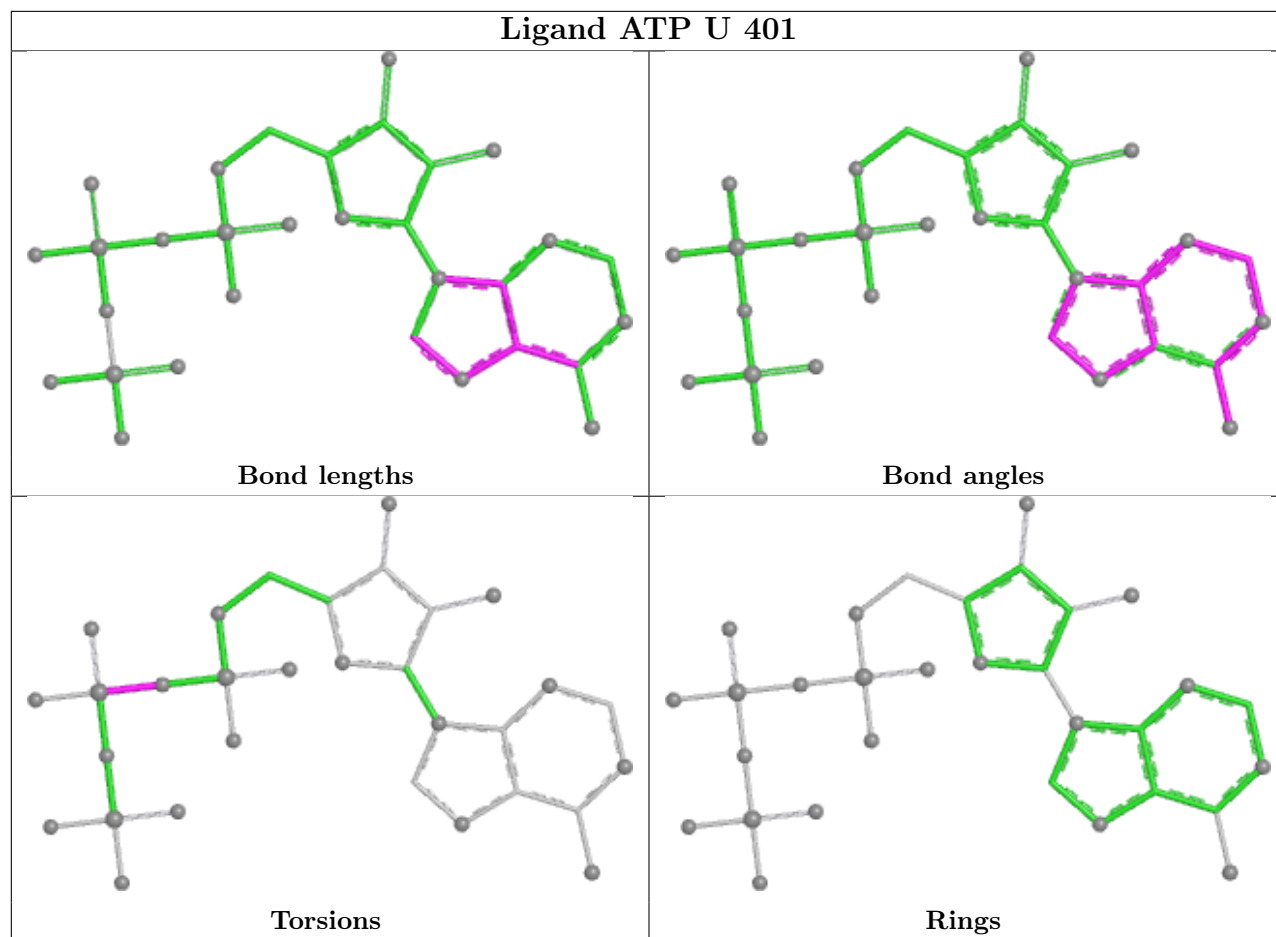


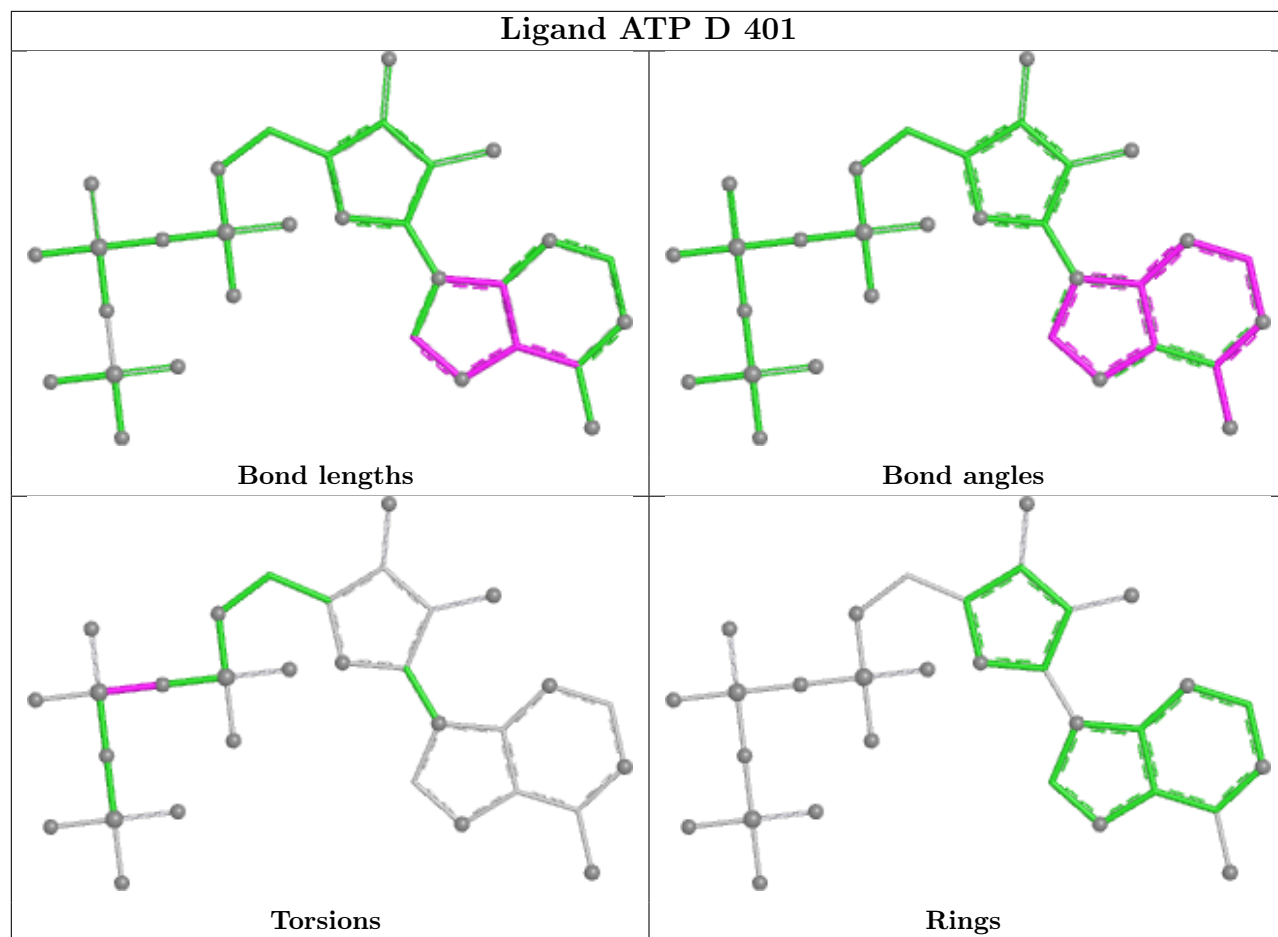


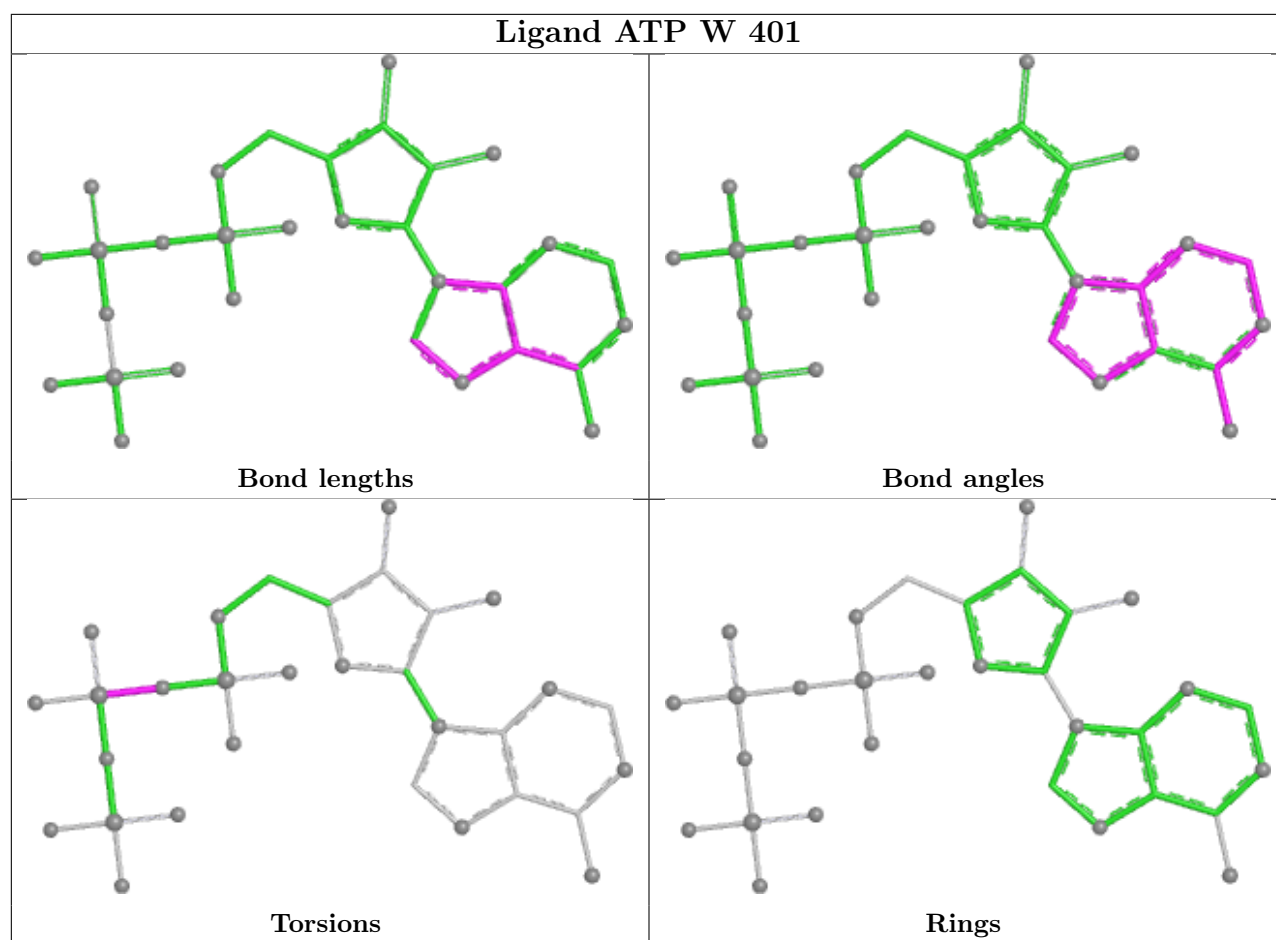


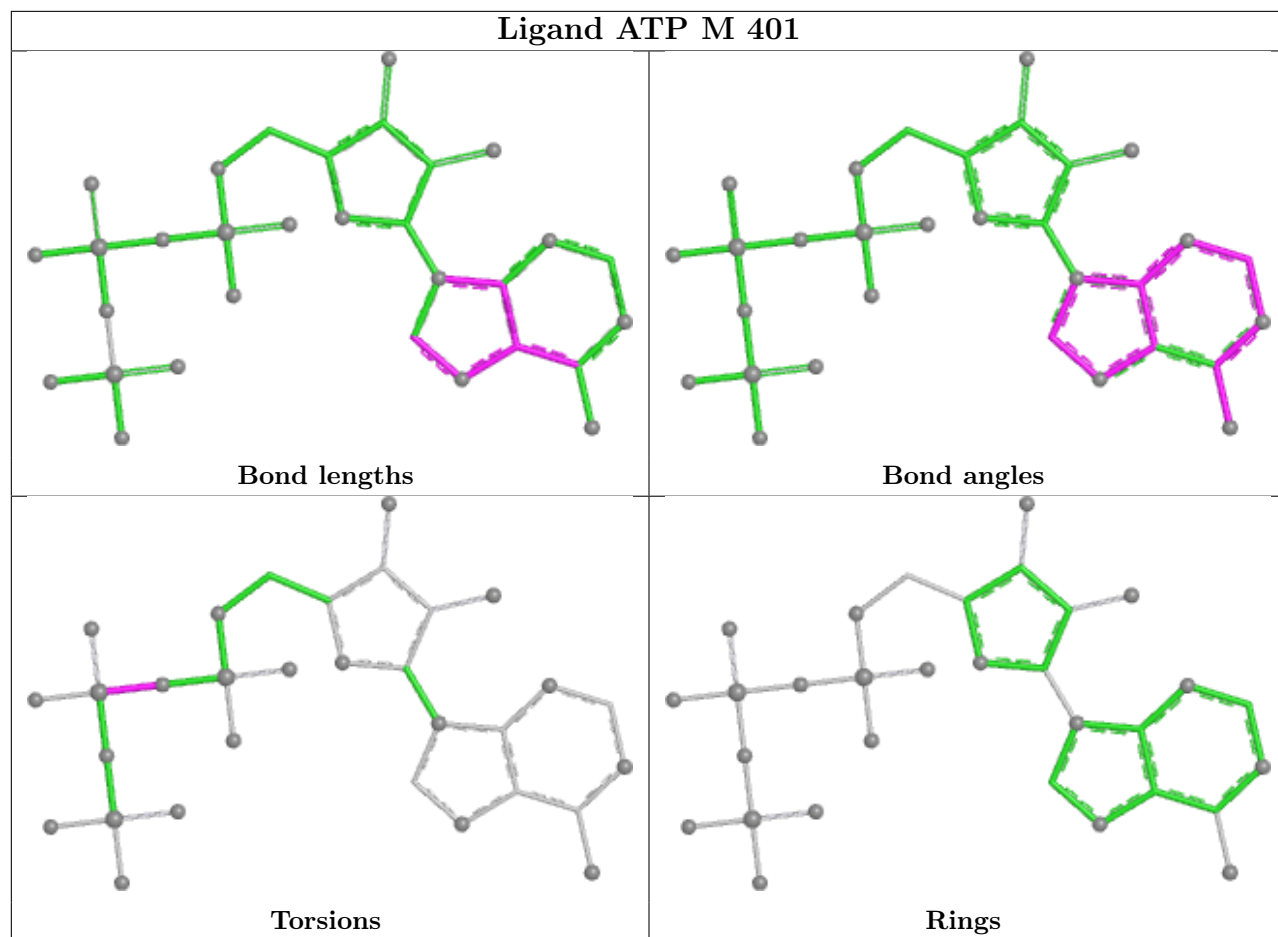


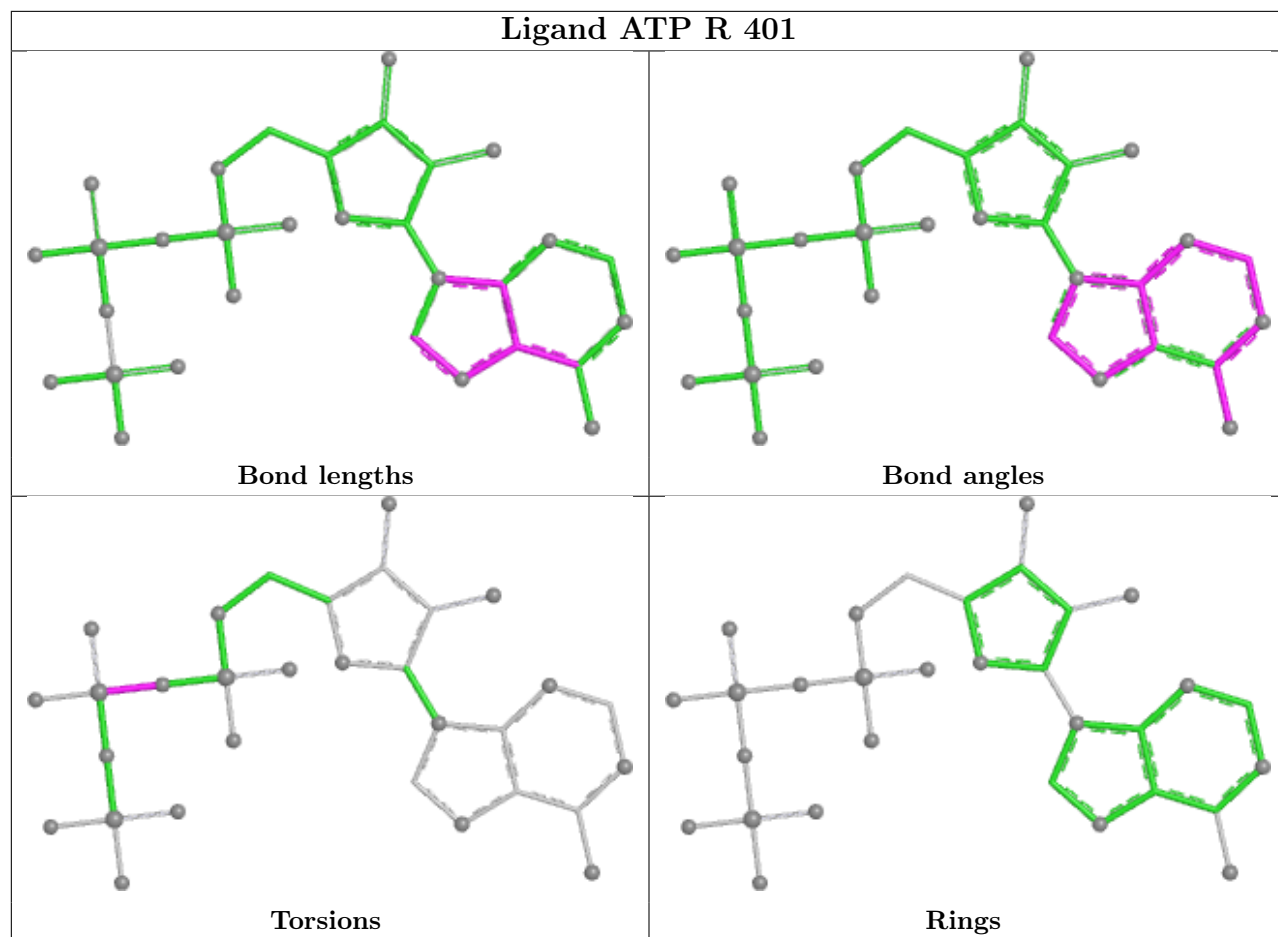


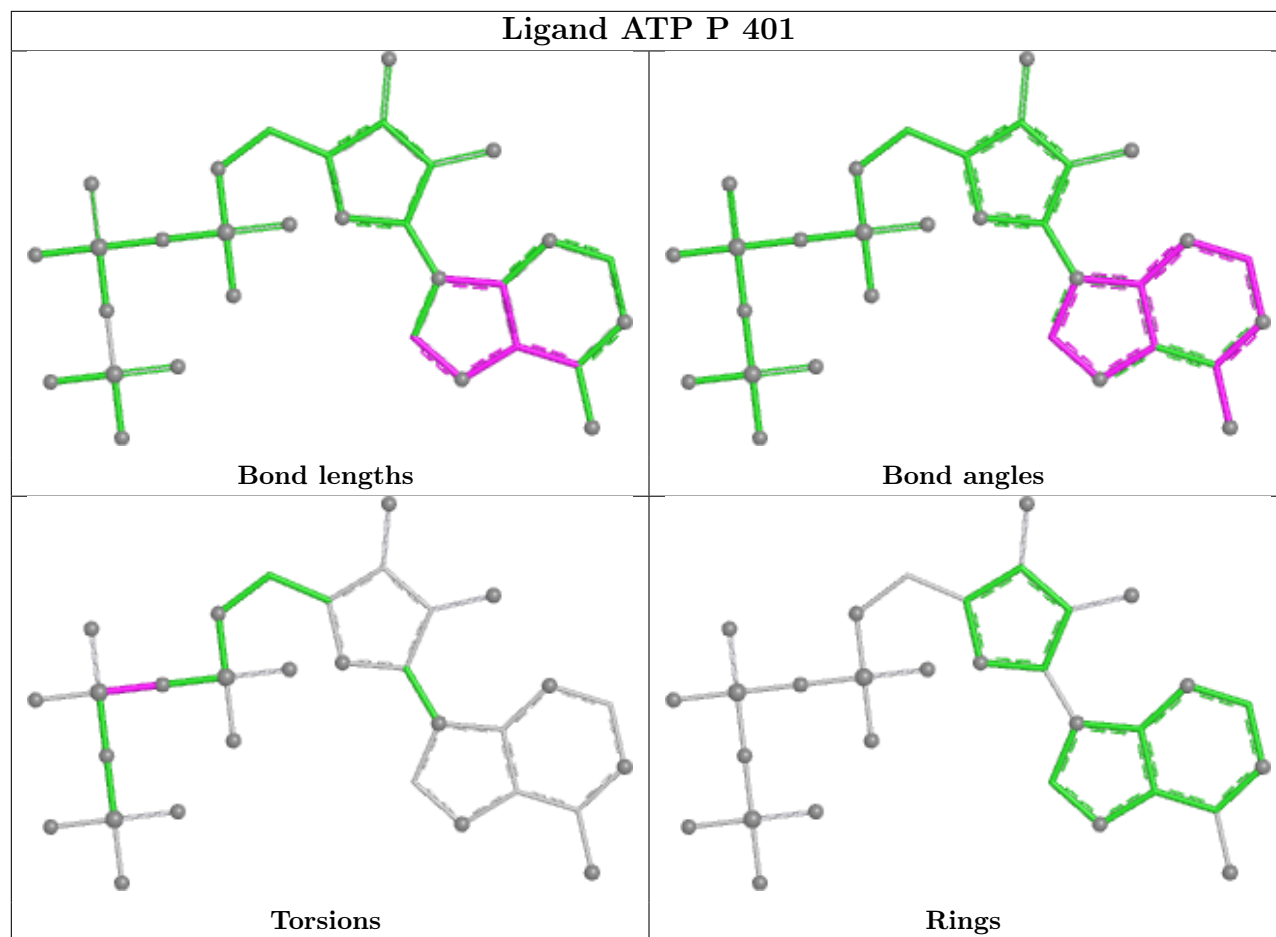


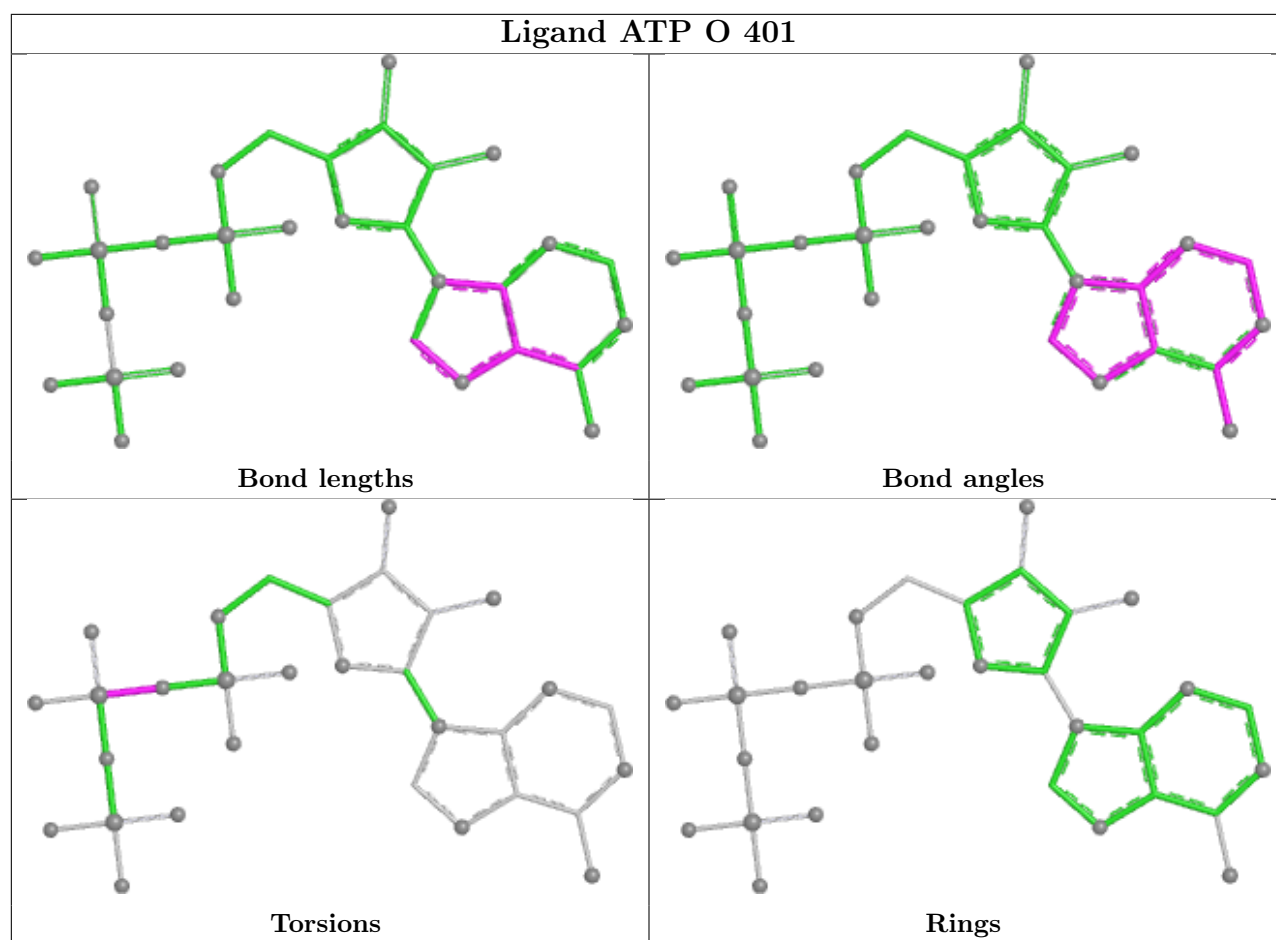


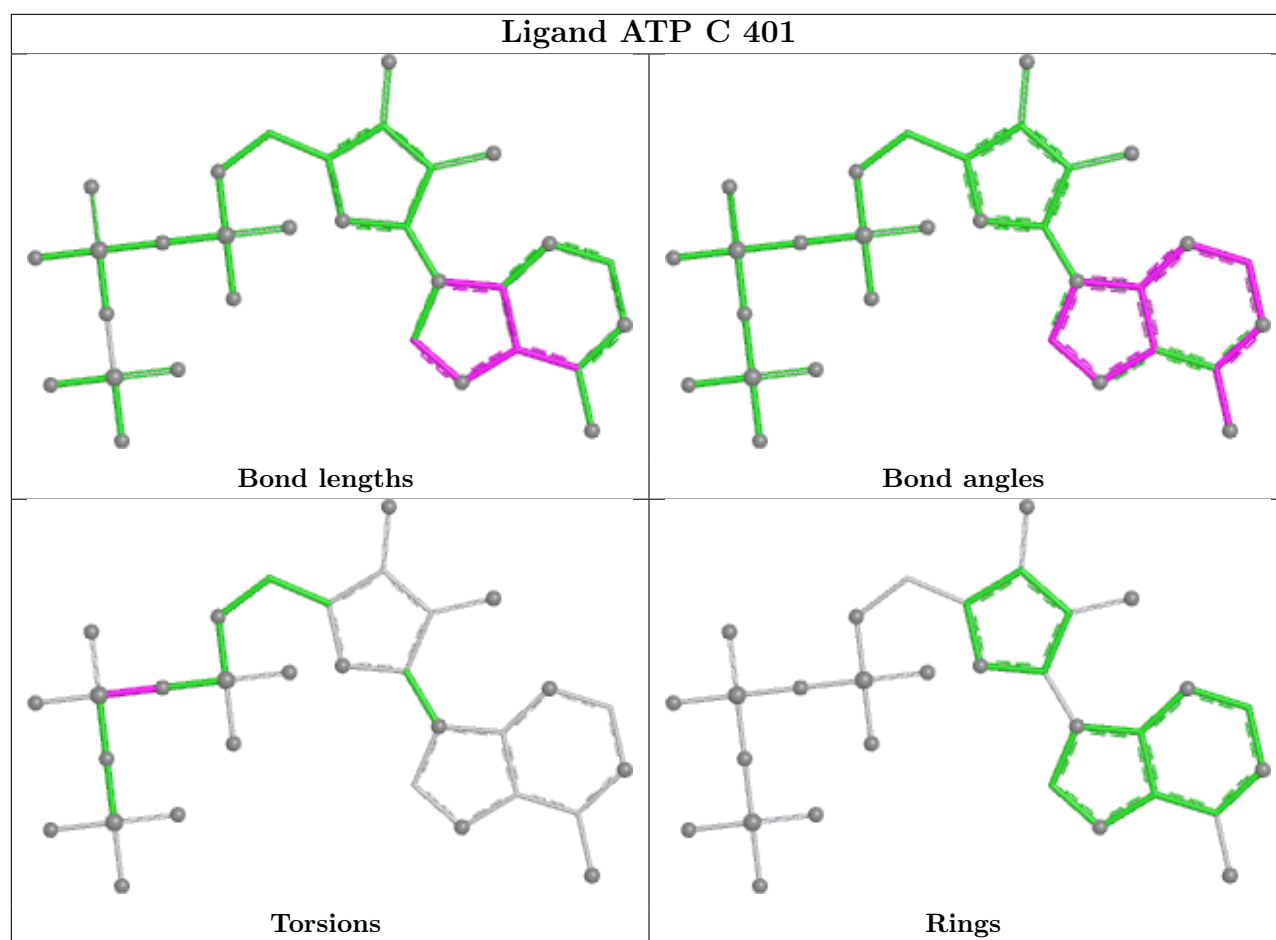












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

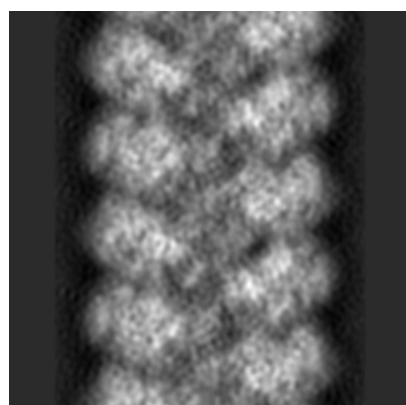
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20076. These allow visual inspection of the internal detail of the map and identification of artifacts.

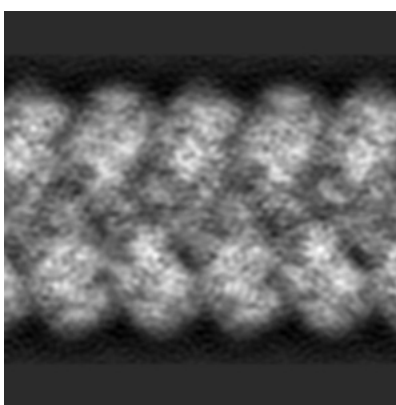
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

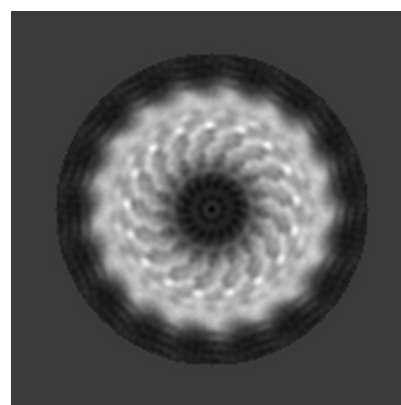
6.1.1 Primary map



X



Y

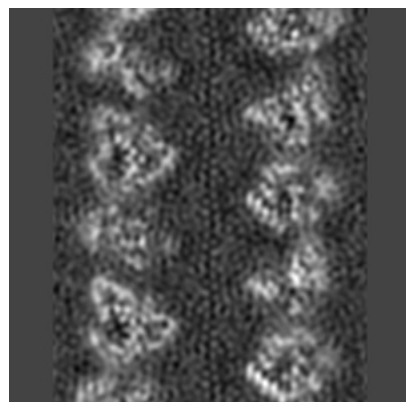


Z

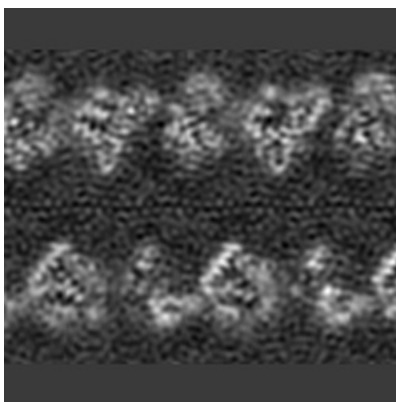
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

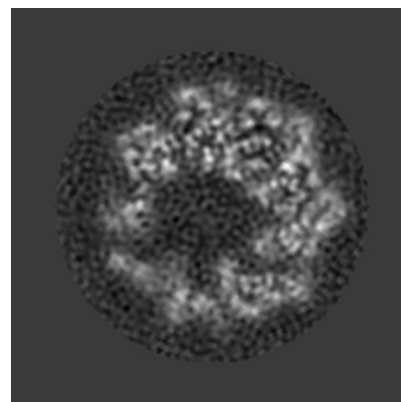
6.2.1 Primary map



X Index: 96



Y Index: 96

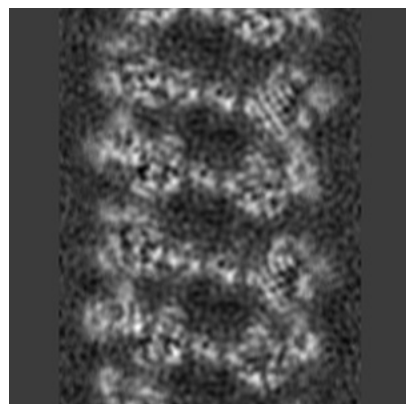


Z Index: 96

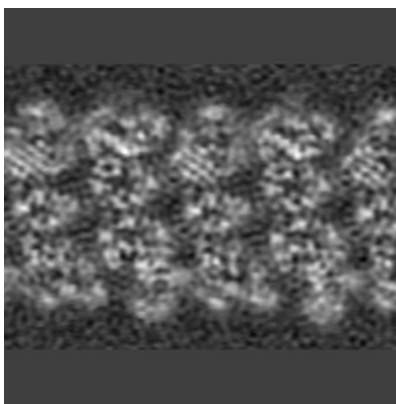
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

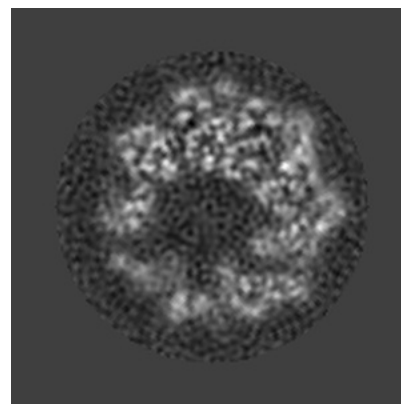
6.3.1 Primary map



X Index: 75



Y Index: 127

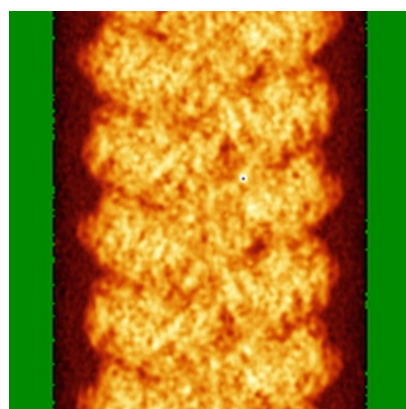


Z Index: 97

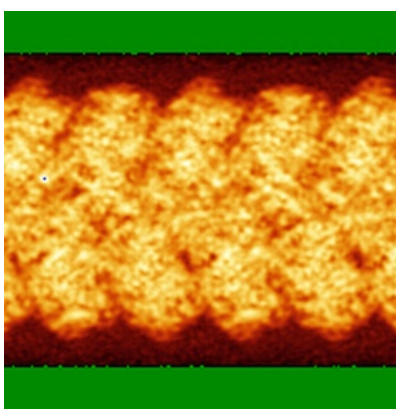
The images above show the largest variance slices of the map in three orthogonal directions.

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

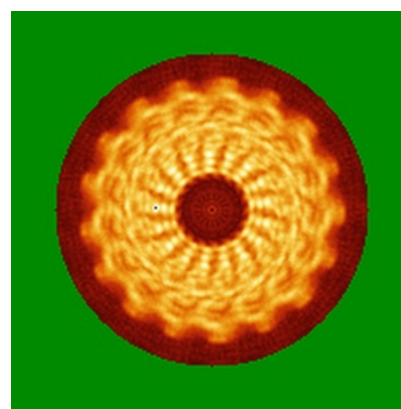
6.4.1 Primary map



X



Y

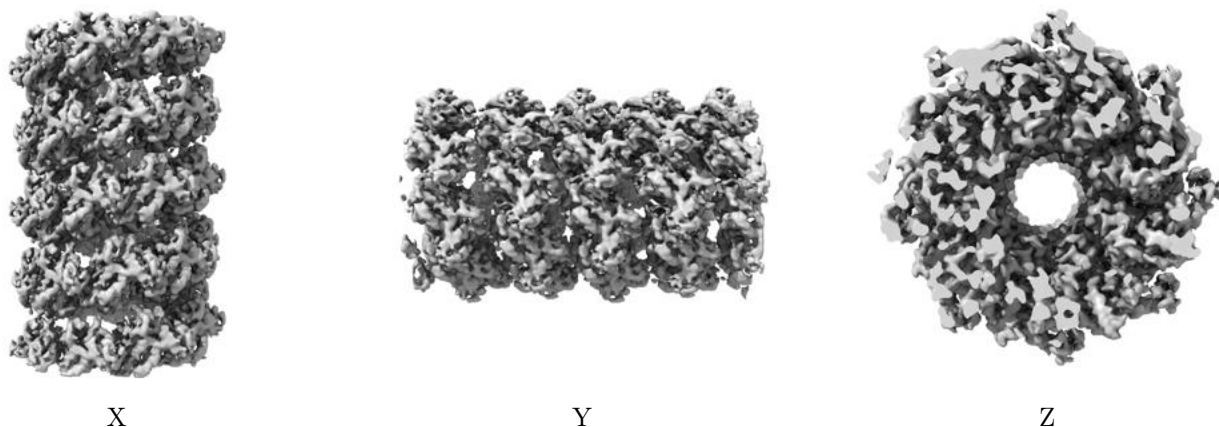


Z

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 0.247. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

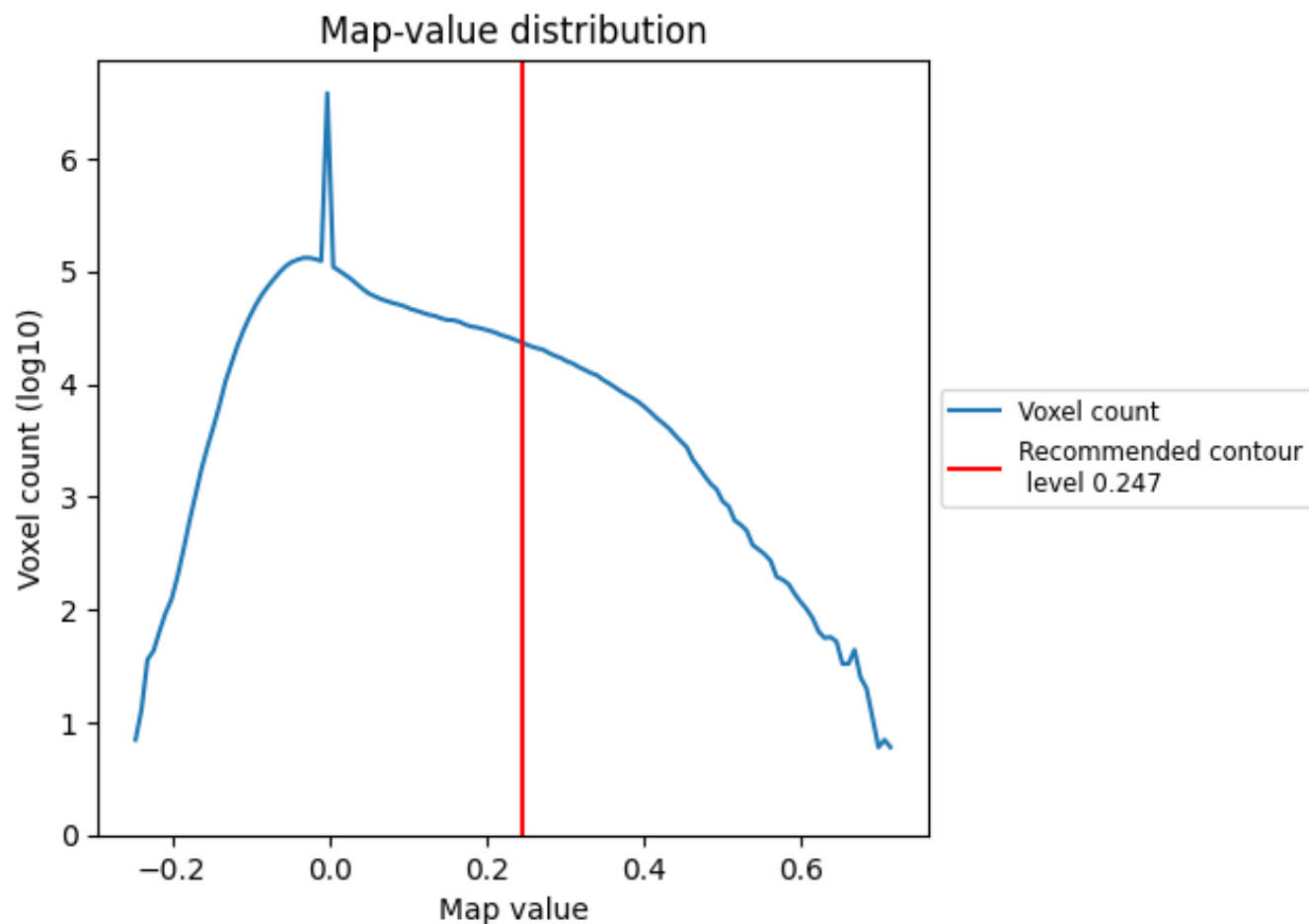
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

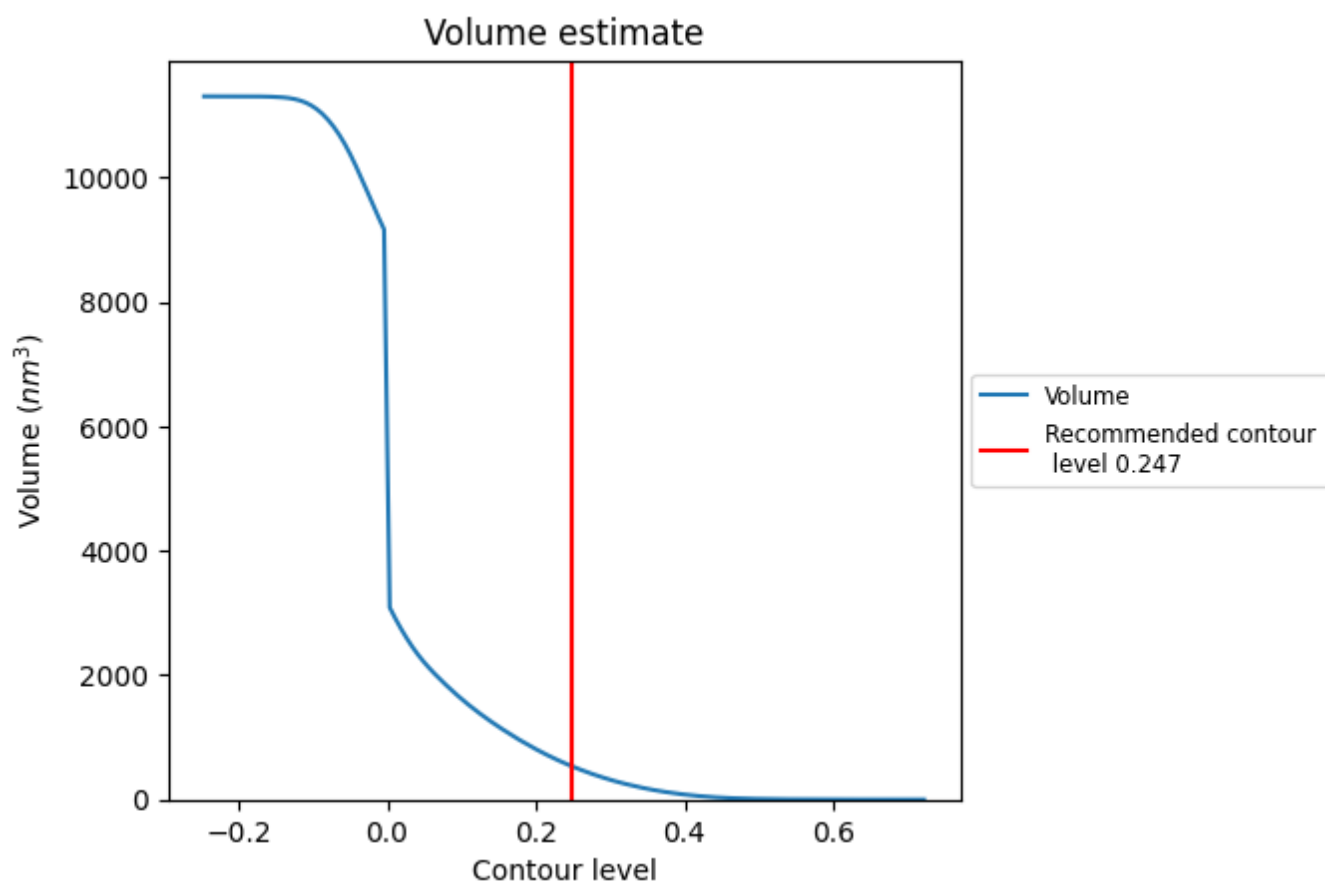
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

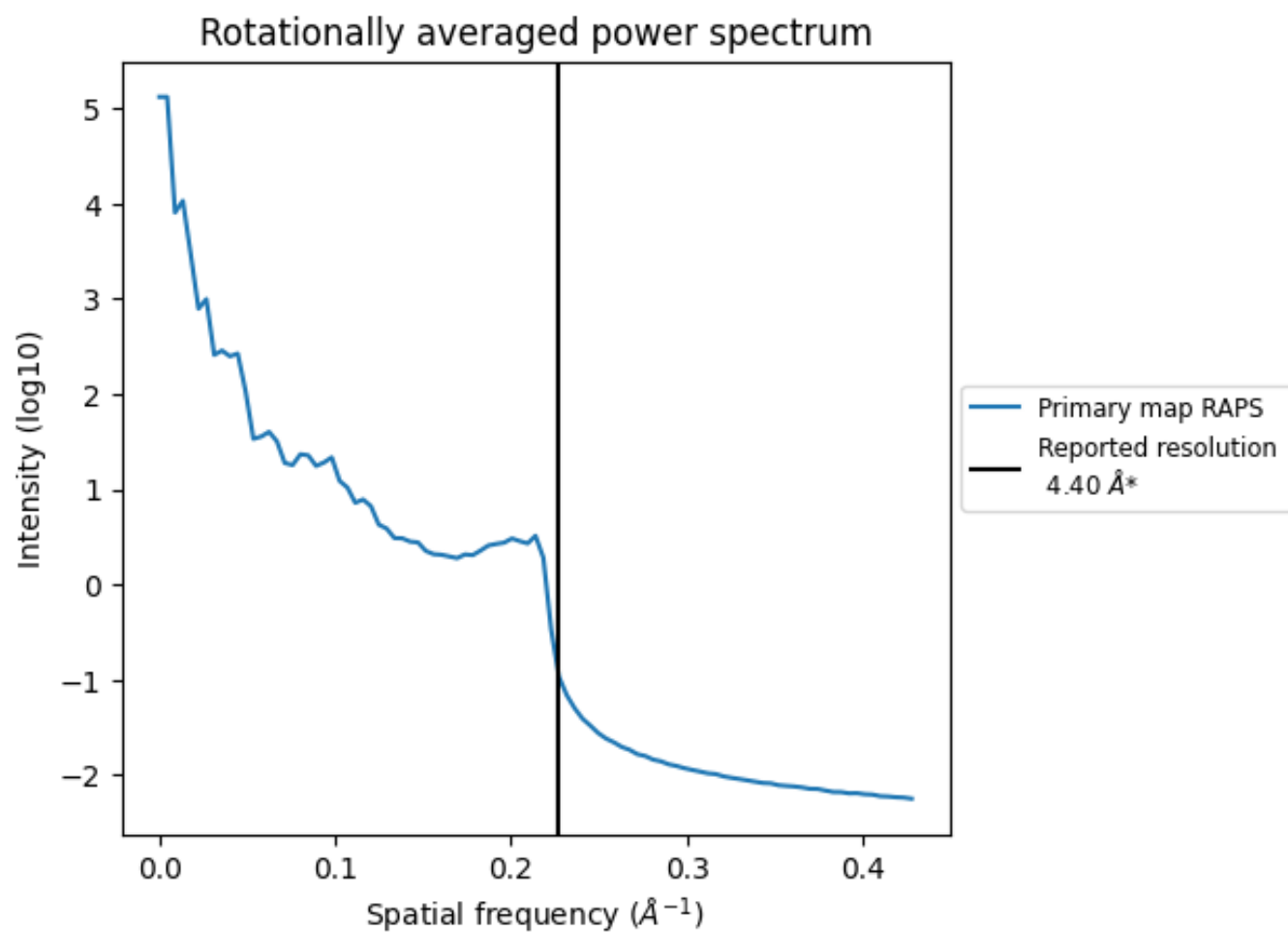
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 543 nm³; this corresponds to an approximate mass of 491 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 0.227 Å⁻¹

8 Fourier-Shell correlation

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

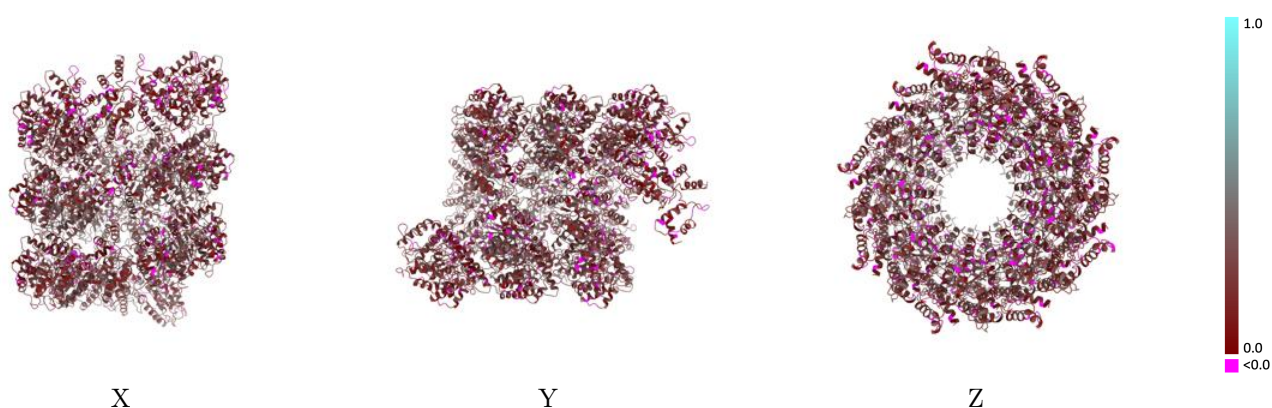
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20076 and PDB model 6OIF. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

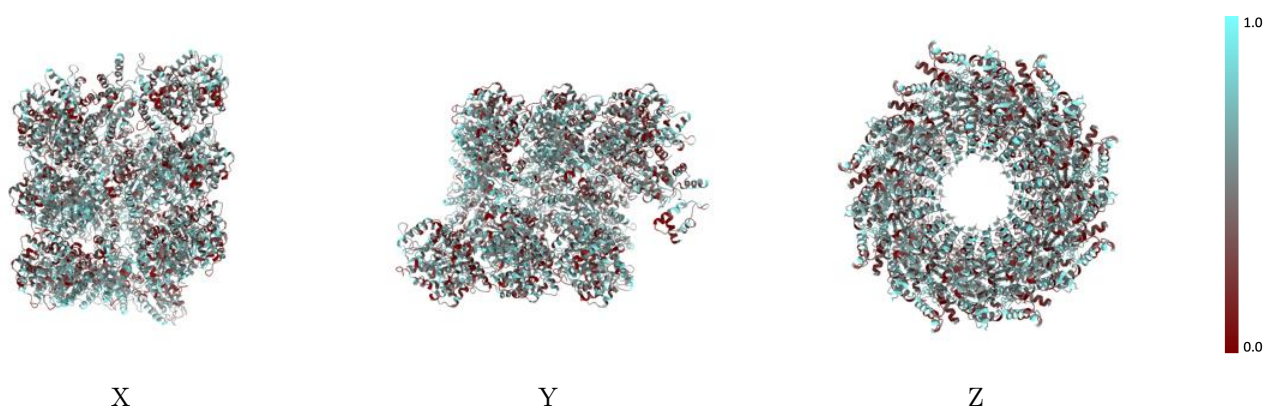
This section was not generated.

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



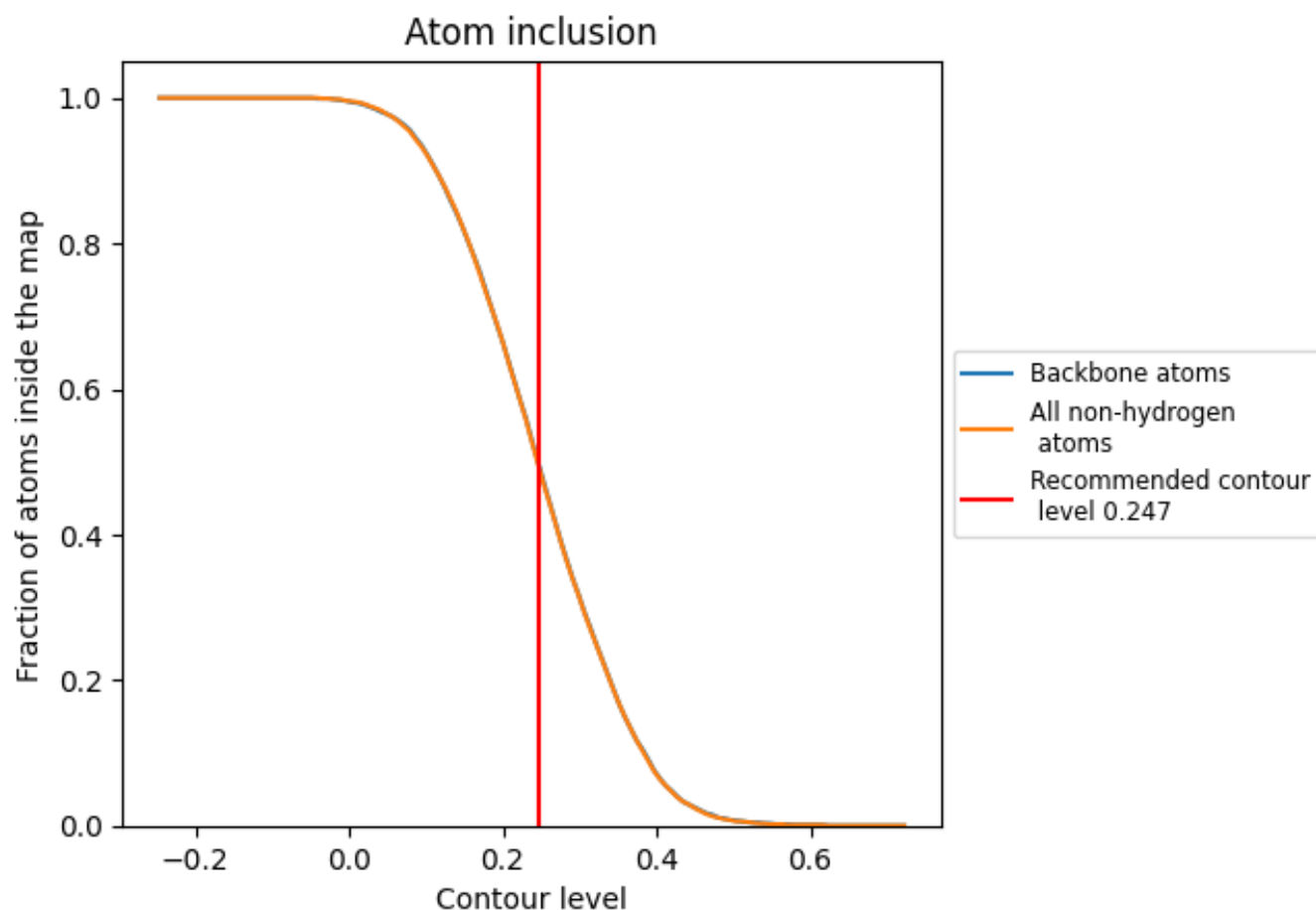
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.247).

9.4 Atom inclusion [i](#)



At the recommended contour level, 50% of all backbone atoms, 49% 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 (0.247) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4930	 0.2210
A	 0.5390	 0.2600
B	 0.5380	 0.2550
C	 0.5400	 0.2560
D	 0.5330	 0.2530
E	 0.5350	 0.2550
F	 0.5210	 0.2460
G	 0.5290	 0.2550
H	 0.5210	 0.2430
I	 0.5270	 0.2490
J	 0.5070	 0.2340
K	 0.5230	 0.2440
L	 0.5080	 0.2240
M	 0.5120	 0.2400
N	 0.5060	 0.2140
O	 0.5080	 0.2290
P	 0.4970	 0.2020
Q	 0.4990	 0.2200
R	 0.4790	 0.1890
S	 0.4860	 0.2090
T	 0.4730	 0.1800
U	 0.4820	 0.1990
V	 0.4530	 0.1650
W	 0.4750	 0.1880
X	 0.4440	 0.1510
Y	 0.4470	 0.1730

