



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 08:59 AM UTC

PDB ID : 7RS6 / pdb_00007rs6
EMDB ID : EMD-24667
Title : Cryo-EM structure of Kip3 (AMPPNP) bound to GMPCPP-Stabilized Microtubules
Authors : Hernandez-Lopez, R.A.; Leschziner, A.E.; Arellano-Santoyo, H.; Pellman, D.; Stokasimov, E.; Wang, R.Y.-R.
Deposited on : 2021-08-11
Resolution : 4.10 Å (reported)
Based on initial models : 4FRZ, 3JAT

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

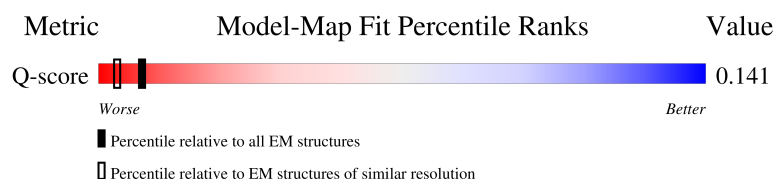
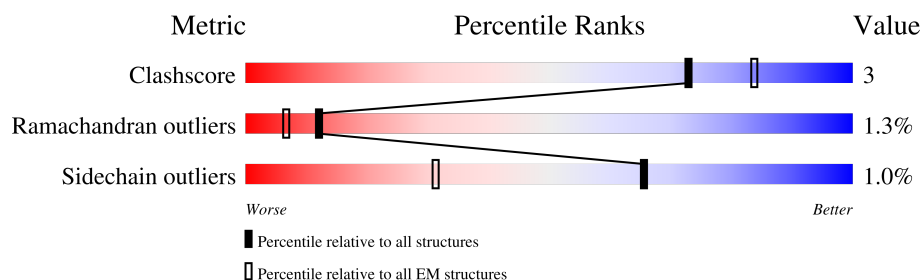
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 4.10 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	6458 (3.60 - 4.60)

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	451	9% 89% 5%
1	C	451	10% 88% 5% • 5%
1	E	451	10% 89% 5% • 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	451	
1	I	451	
1	L	451	
1	N	451	
1	P	451	
1	R	451	
2	B	445	
2	D	445	
2	F	445	
2	H	445	
2	J	445	
2	M	445	
2	O	445	
2	Q	445	
2	S	445	
3	K	355	
3	a	355	
3	b	355	
3	c	355	
3	d	355	
3	e	355	
3	f	355	
3	g	355	
3	h	355	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 166941 atoms, of which 82413 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 Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	428	Total	C	H	N	O	S	0	0
			6634	2130	3276	571	635	22		
1	C	428	Total	C	H	N	O	S	0	0
			6634	2130	3276	571	635	22		
1	E	428	Total	C	H	N	O	S	0	0
			6634	2130	3276	571	635	22		
1	G	428	Total	C	H	N	O	S	0	0
			6634	2130	3276	571	635	22		
1	I	428	Total	C	H	N	O	S	0	0
			6634	2130	3276	571	635	22		
1	L	428	Total	C	H	N	O	S	0	0
			6634	2130	3276	571	635	22		
1	N	428	Total	C	H	N	O	S	0	0
			6634	2130	3276	571	635	22		
1	P	428	Total	C	H	N	O	S	0	0
			6634	2130	3276	571	635	22		
1	R	428	Total	C	H	N	O	S	0	0
			6634	2130	3276	571	635	22		

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	426	Total	C	H	N	O	S	0	0
			6586	2106	3235	575	644	26		
2	D	426	Total	C	H	N	O	S	0	0
			6586	2106	3235	575	644	26		
2	F	426	Total	C	H	N	O	S	0	0
			6586	2106	3235	575	644	26		
2	H	426	Total	C	H	N	O	S	0	0
			6586	2106	3235	575	644	26		
2	J	426	Total	C	H	N	O	S	0	0
			6586	2106	3235	575	644	26		
2	M	426	Total	C	H	N	O	S	0	0
			6586	2106	3235	575	644	26		

Continued on next page...

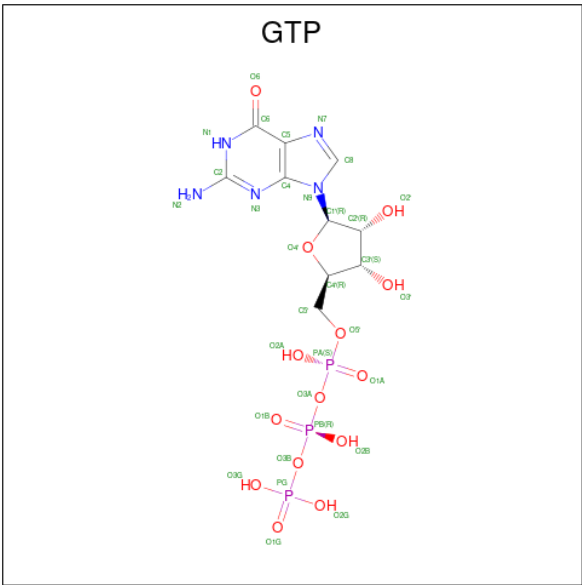
Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf	Trace
2	O	426	Total	C	H	N	O	S	0	0
			6586	2106	3235	575	644	26		
2	Q	426	Total	C	H	N	O	S	0	0
			6586	2106	3235	575	644	26		
2	S	426	Total	C	H	N	O	S	0	0
			6586	2106	3235	575	644	26		

- Molecule 3 is a protein called kinesin-8/ Kip3.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	K	330	Total	C	H	N	O	S	0	0
			5192	1616	2607	457	499	13		
3	a	330	Total	C	H	N	O	S	0	0
			5192	1616	2607	457	499	13		
3	b	330	Total	C	H	N	O	S	0	0
			5192	1616	2607	457	499	13		
3	c	330	Total	C	H	N	O	S	0	0
			5192	1616	2607	457	499	13		
3	d	330	Total	C	H	N	O	S	0	0
			5192	1616	2607	457	499	13		
3	e	330	Total	C	H	N	O	S	0	0
			5192	1616	2607	457	499	13		
3	f	330	Total	C	H	N	O	S	0	0
			5192	1616	2607	457	499	13		
3	g	330	Total	C	H	N	O	S	0	0
			5192	1616	2607	457	499	13		
3	h	330	Total	C	H	N	O	S	0	0
			5192	1616	2607	457	499	13		

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
4	A	1	Total	C	H	N	O	P	0
			44	10	12	5	14	3	
4	C	1	Total	C	H	N	O	P	0
			44	10	12	5	14	3	
4	E	1	Total	C	H	N	O	P	0
			44	10	12	5	14	3	
4	G	1	Total	C	H	N	O	P	0
			44	10	12	5	14	3	
4	I	1	Total	C	H	N	O	P	0
			44	10	12	5	14	3	
4	L	1	Total	C	H	N	O	P	0
			44	10	12	5	14	3	
4	N	1	Total	C	H	N	O	P	0
			44	10	12	5	14	3	
4	P	1	Total	C	H	N	O	P	0
			44	10	12	5	14	3	
4	R	1	Total	C	H	N	O	P	0
			44	10	12	5	14	3	

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Mg	0
			1	1	
5	B	1	Total	Mg	0
			1	1	

Continued on next page...

Continued from previous page...

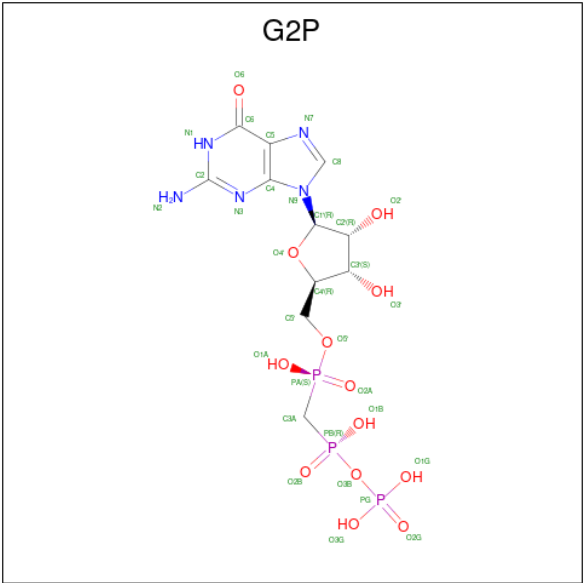
Mol	Chain	Residues	Atoms		AltConf
5	K	1	Total 1	Mg 1	0
5	C	1	Total 1	Mg 1	0
5	D	1	Total 1	Mg 1	0
5	a	1	Total 1	Mg 1	0
5	E	1	Total 1	Mg 1	0
5	F	1	Total 1	Mg 1	0
5	b	1	Total 1	Mg 1	0
5	G	1	Total 1	Mg 1	0
5	H	1	Total 1	Mg 1	0
5	c	1	Total 1	Mg 1	0
5	I	1	Total 1	Mg 1	0
5	J	1	Total 1	Mg 1	0
5	d	1	Total 1	Mg 1	0
5	L	1	Total 1	Mg 1	0
5	M	1	Total 1	Mg 1	0
5	e	1	Total 1	Mg 1	0
5	N	1	Total 1	Mg 1	0
5	O	1	Total 1	Mg 1	0
5	f	1	Total 1	Mg 1	0
5	P	1	Total 1	Mg 1	0
5	Q	1	Total 1	Mg 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
5	g	1	Total	Mg	0
			1	1	
5	R	1	Total	Mg	0
			1	1	
5	S	1	Total	Mg	0
			1	1	
5	h	1	Total	Mg	0
			1	1	

- Molecule 6 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: G2P) (formula: C₁₁H₁₈N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



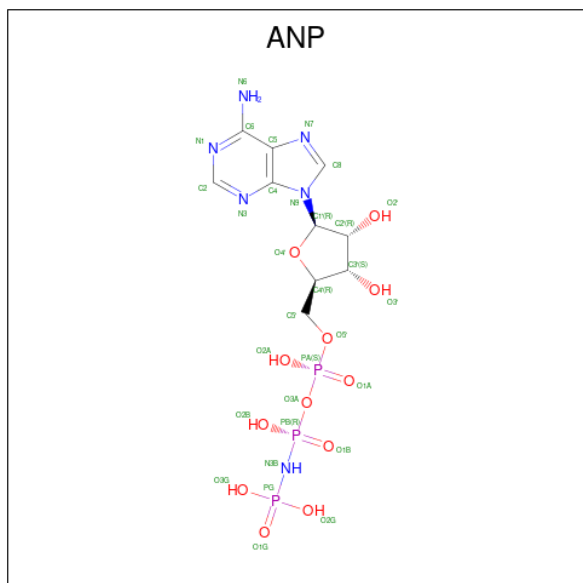
Mol	Chain	Residues	Atoms						AltConf
6	B	1	Total	C	H	N	O	P	0
			46	11	14	5	13	3	
6	D	1	Total	C	H	N	O	P	0
			46	11	14	5	13	3	
6	F	1	Total	C	H	N	O	P	0
			46	11	14	5	13	3	
6	H	1	Total	C	H	N	O	P	0
			46	11	14	5	13	3	
6	J	1	Total	C	H	N	O	P	0
			46	11	14	5	13	3	
6	M	1	Total	C	H	N	O	P	0
			46	11	14	5	13	3	
6	O	1	Total	C	H	N	O	P	0
			46	11	14	5	13	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
6	Q	1	Total	C	H	N	O	P
			46	11	14	5	13	3
6	S	1	Total	C	H	N	O	P
			46	11	14	5	13	3

- Molecule 7 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).

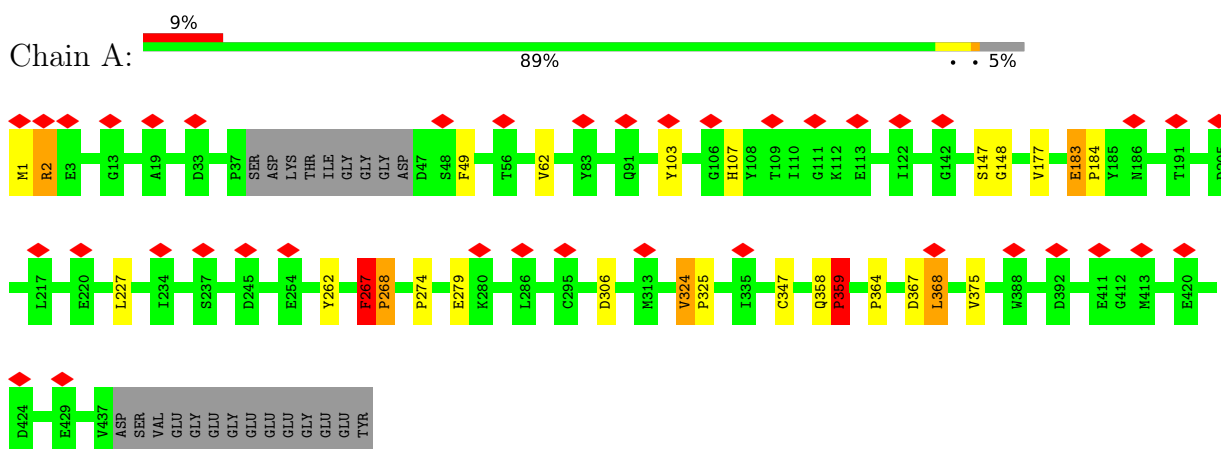


Mol	Chain	Residues	Atoms					AltConf
7	K	1	Total	C	H	N	O	P
			44	10	13	6	12	3
7	a	1	Total	C	H	N	O	P
			44	10	13	6	12	3
7	b	1	Total	C	H	N	O	P
			44	10	13	6	12	3
7	c	1	Total	C	H	N	O	P
			44	10	13	6	12	3
7	d	1	Total	C	H	N	O	P
			44	10	13	6	12	3
7	e	1	Total	C	H	N	O	P
			44	10	13	6	12	3
7	f	1	Total	C	H	N	O	P
			44	10	13	6	12	3
7	g	1	Total	C	H	N	O	P
			44	10	13	6	12	3
7	h	1	Total	C	H	N	O	P
			44	10	13	6	12	3

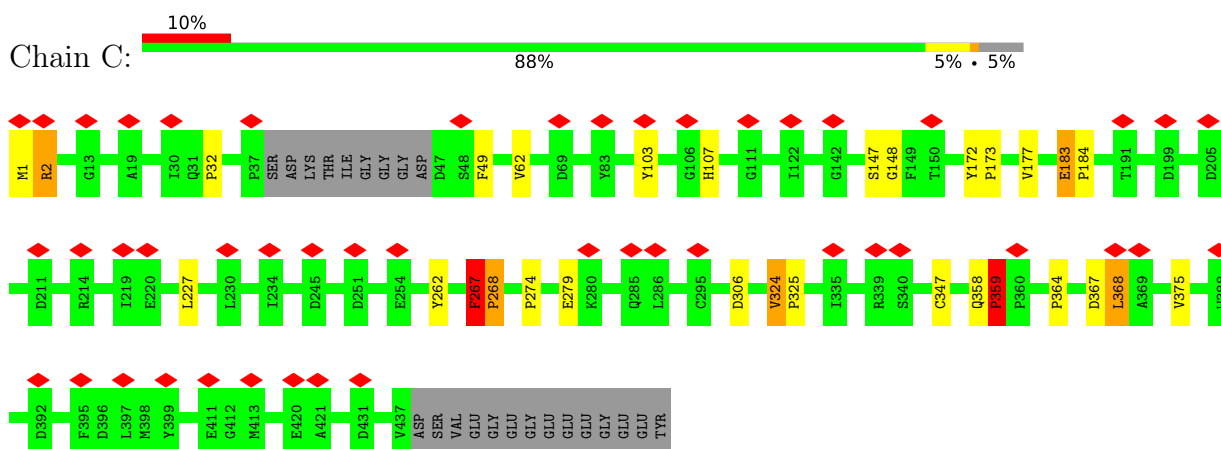
3 Residue-property plots [i](#)

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.

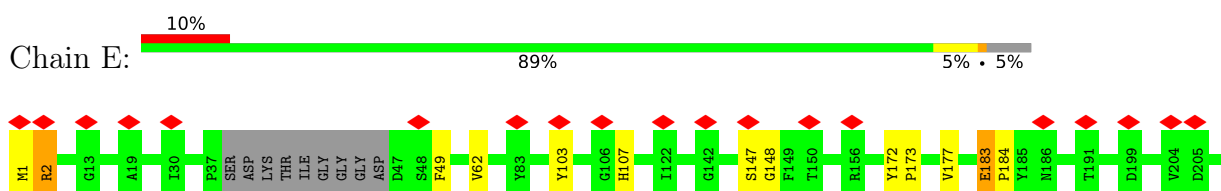
- Molecule 1: Tubulin alpha-1B chain

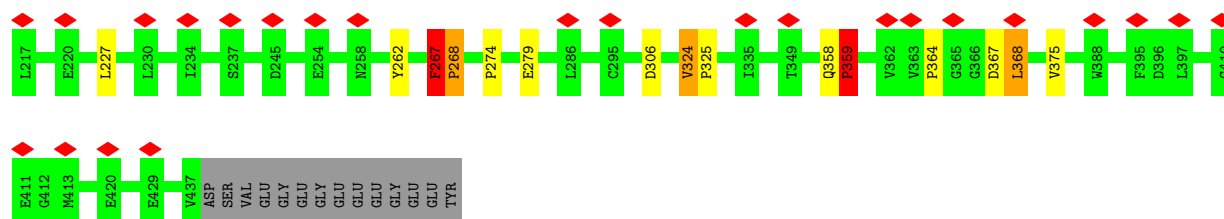


- Molecule 1: Tubulin alpha-1B chain

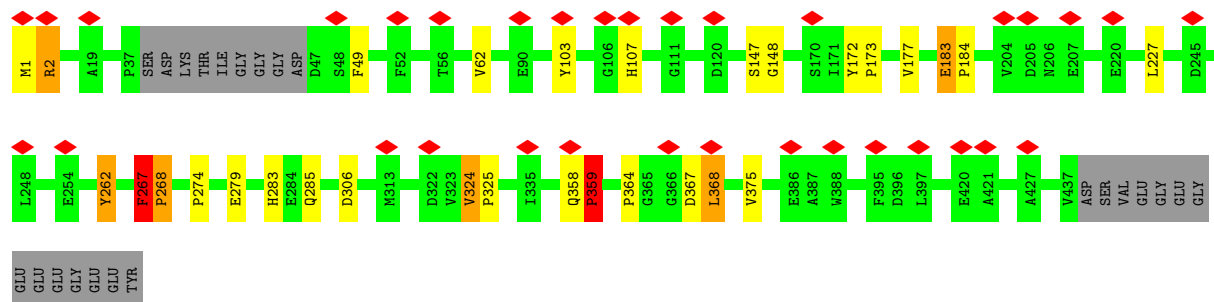
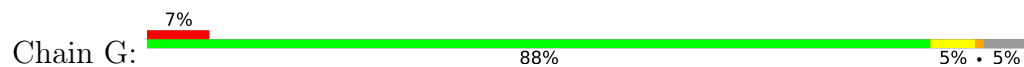


- Molecule 1: Tubulin alpha-1B chain

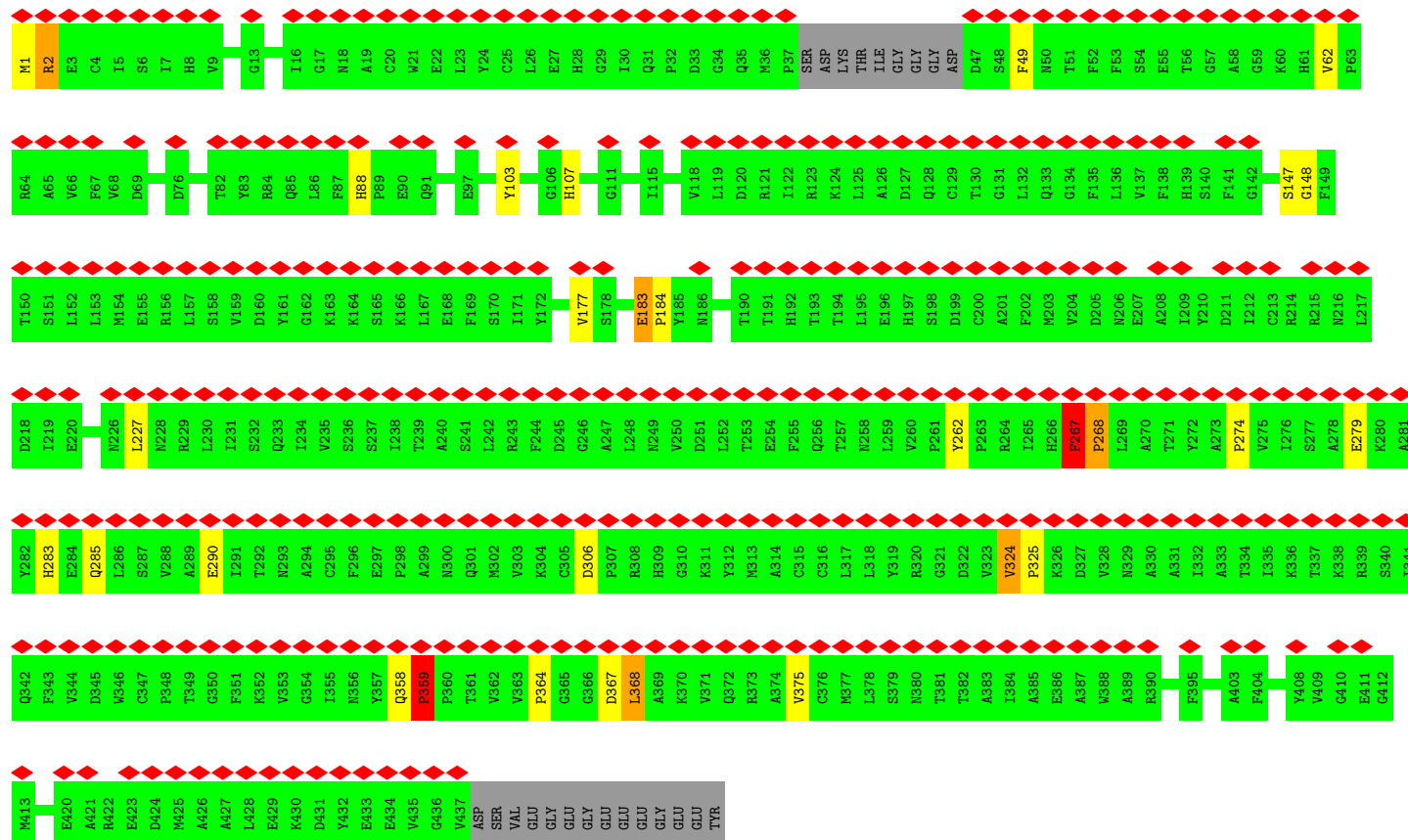
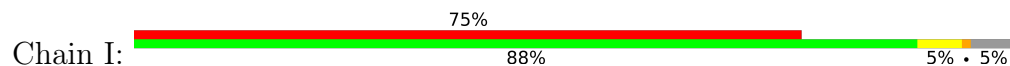




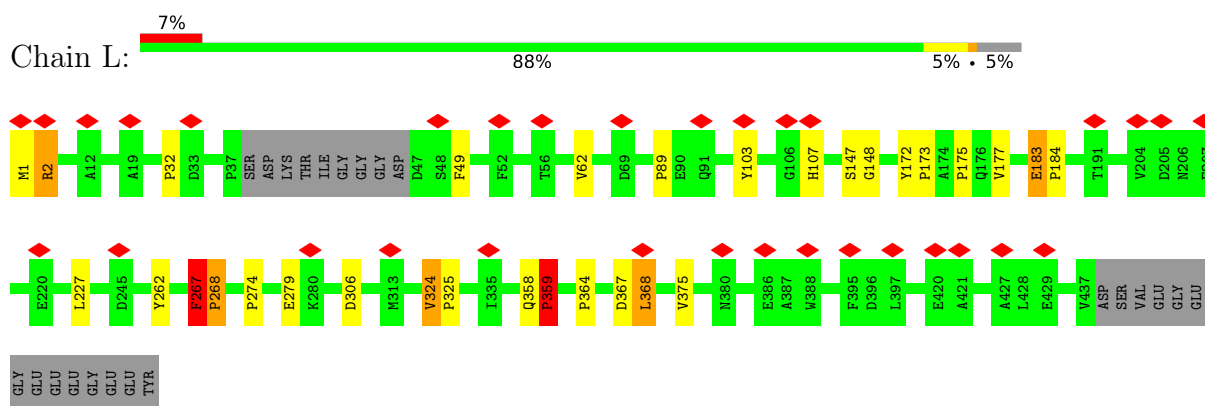
• Molecule 1: Tubulin alpha-1B chain



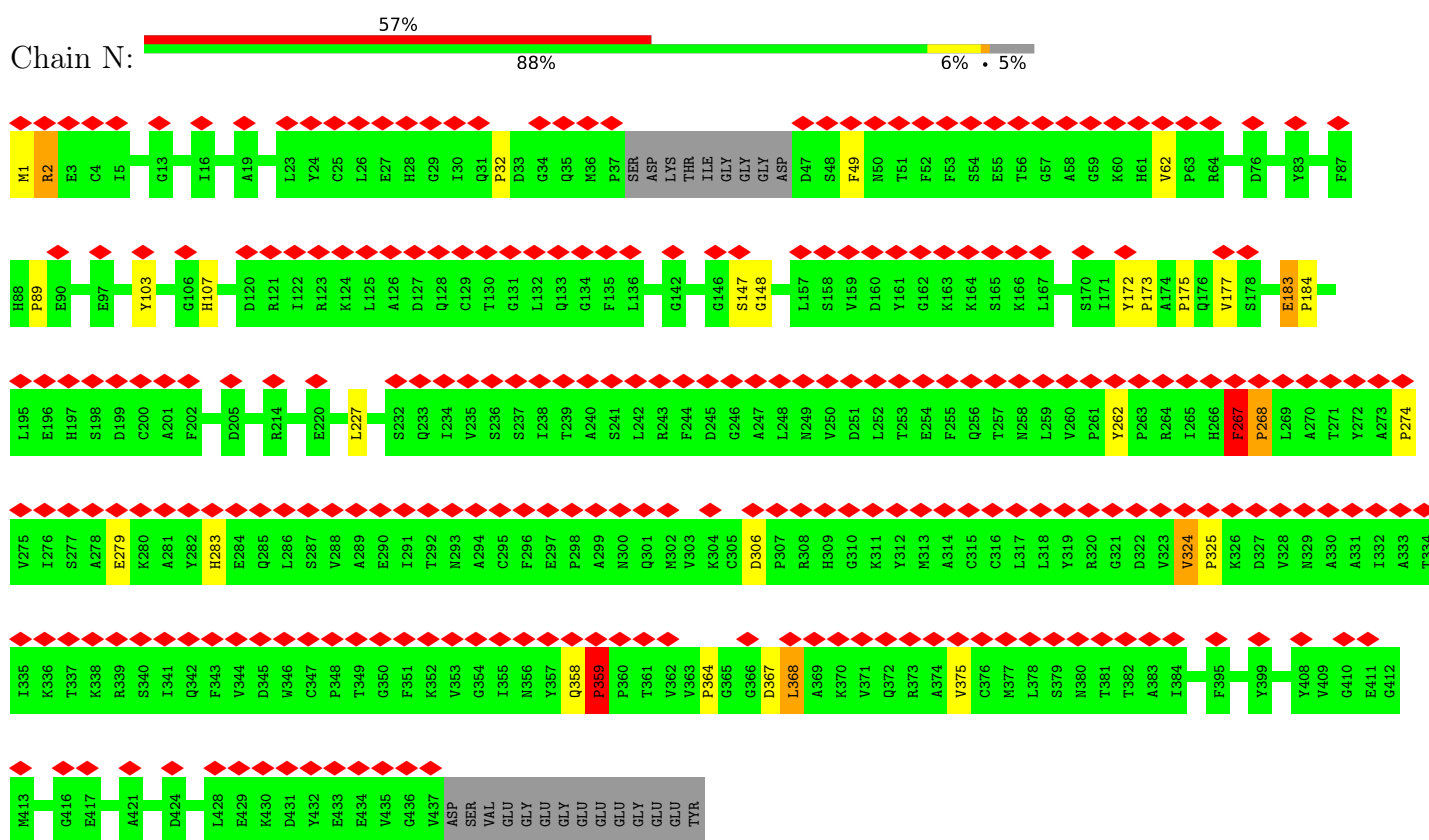
• Molecule 1: Tubulin alpha-1B chain



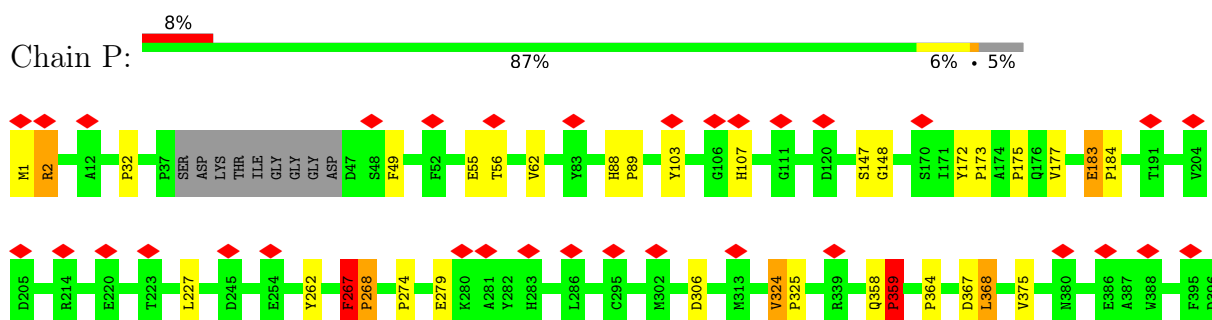
- Molecule 1: Tubulin alpha-1B chain

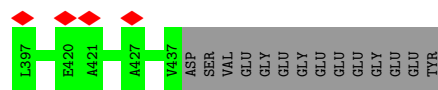


- Molecule 1: Tubulin alpha-1B chain



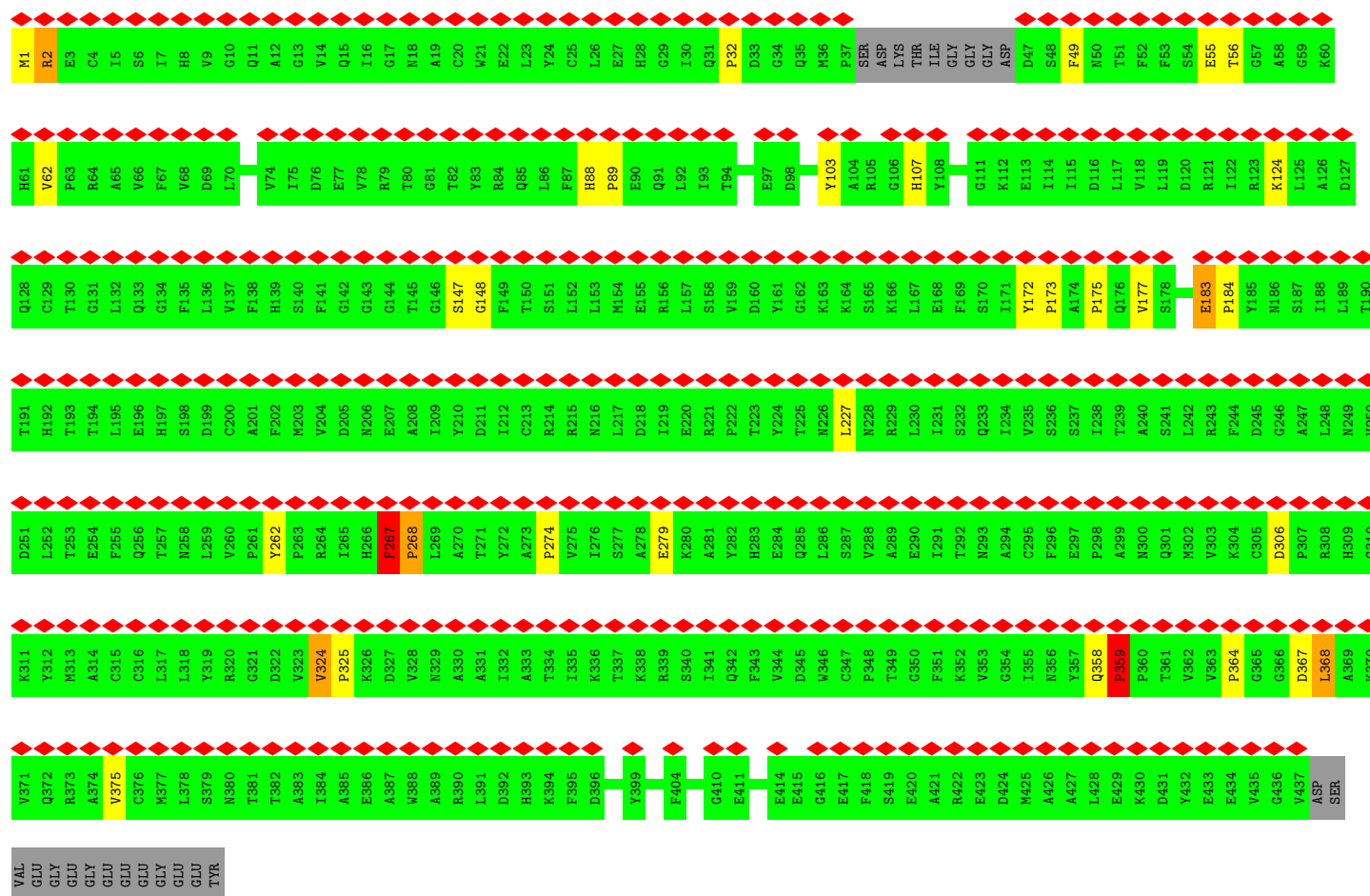
- Molecule 1: Tubulin alpha-1B chain





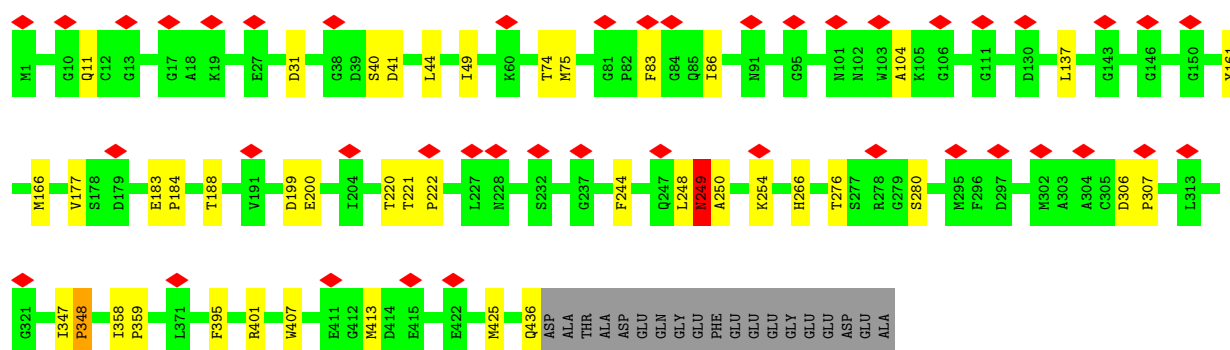
• Molecule 1: Tubulin alpha-1B chain

Chain R: 88%
87% 6% • 5%



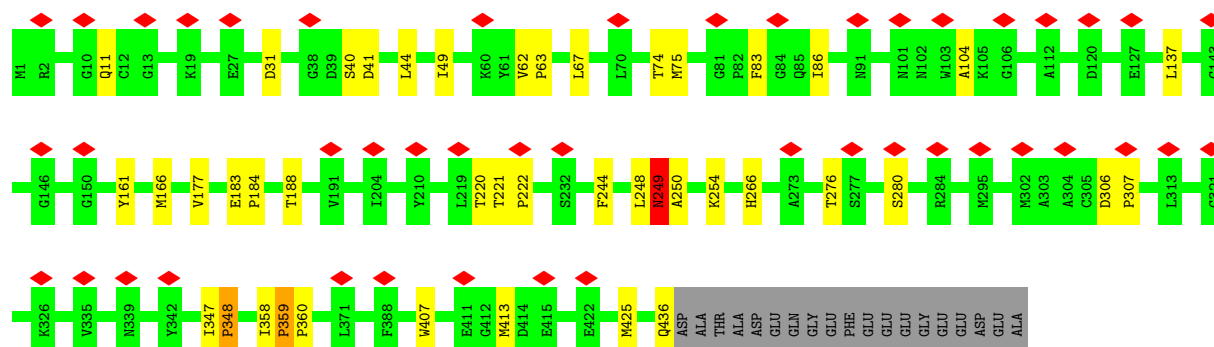
• Molecule 2: Tubulin beta chain

Chain B: 10%
86% 9%



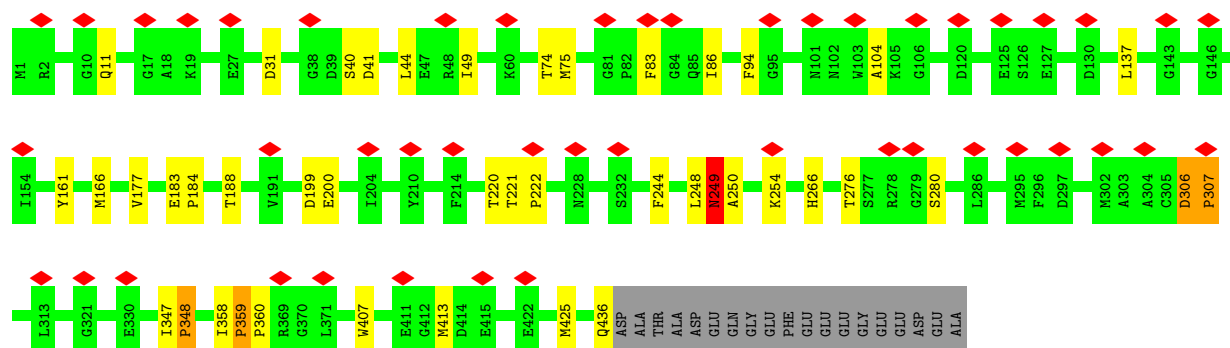
- Molecule 2: Tubulin beta chain

Chain D: 



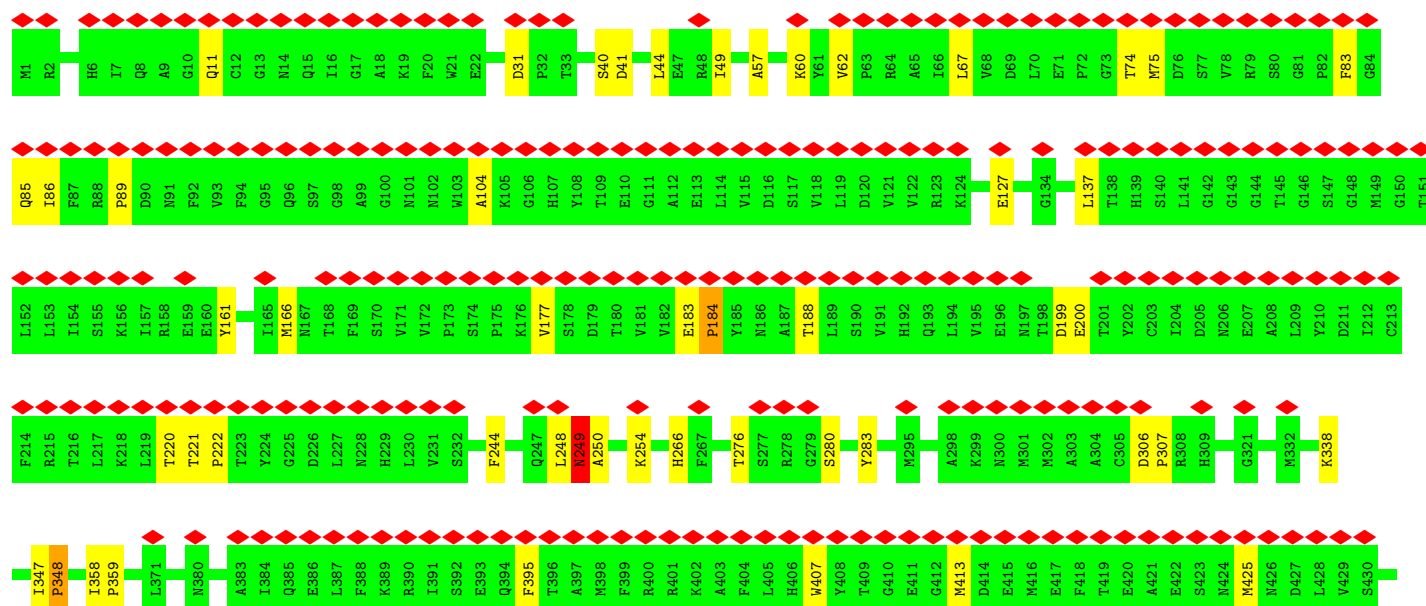
- Molecule 2: Tubulin beta chain

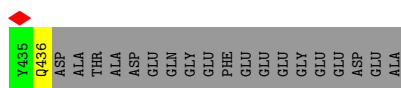
Chain F: 



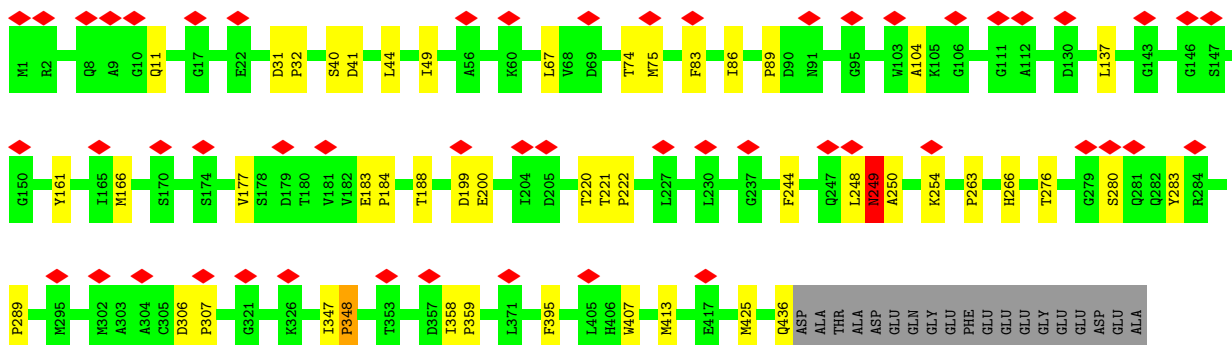
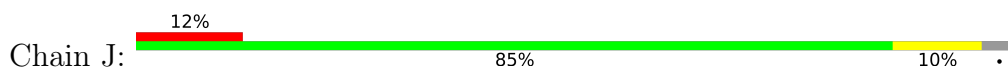
- Molecule 2: Tubulin beta chain

Chain H: 

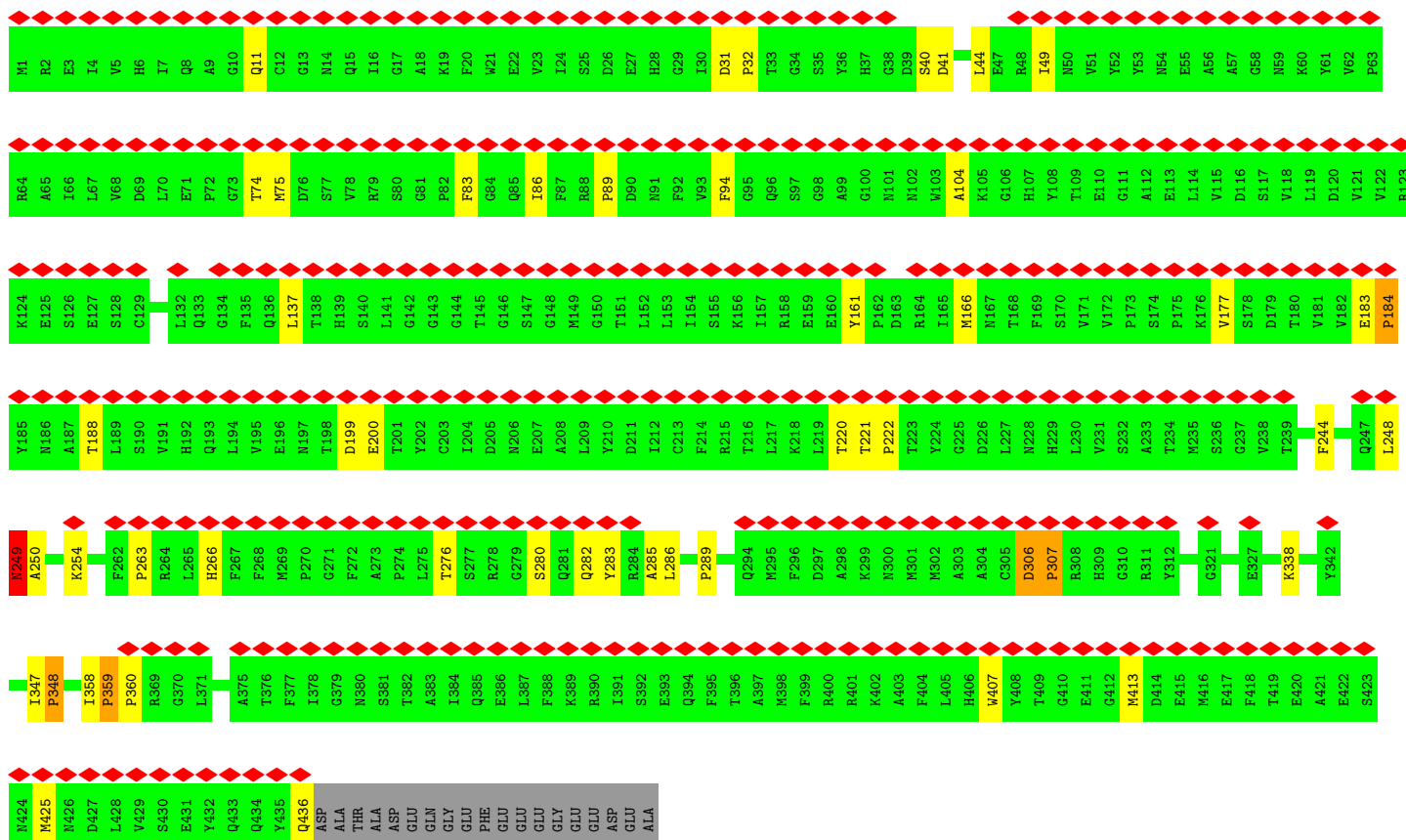
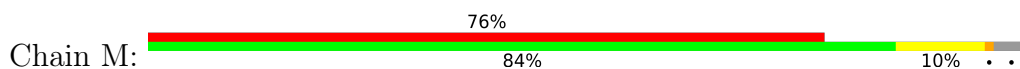




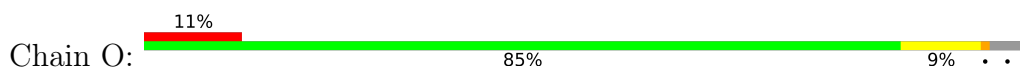
- Molecule 2: Tubulin beta chain

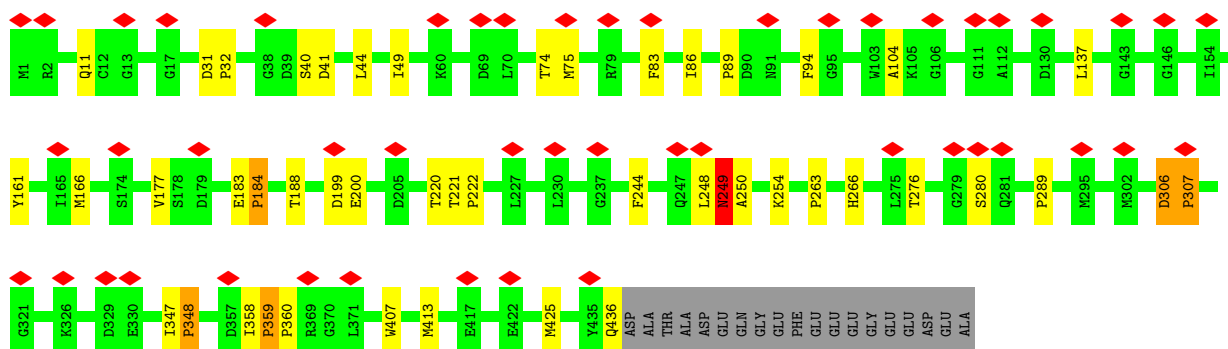


- Molecule 2: Tubulin beta chain

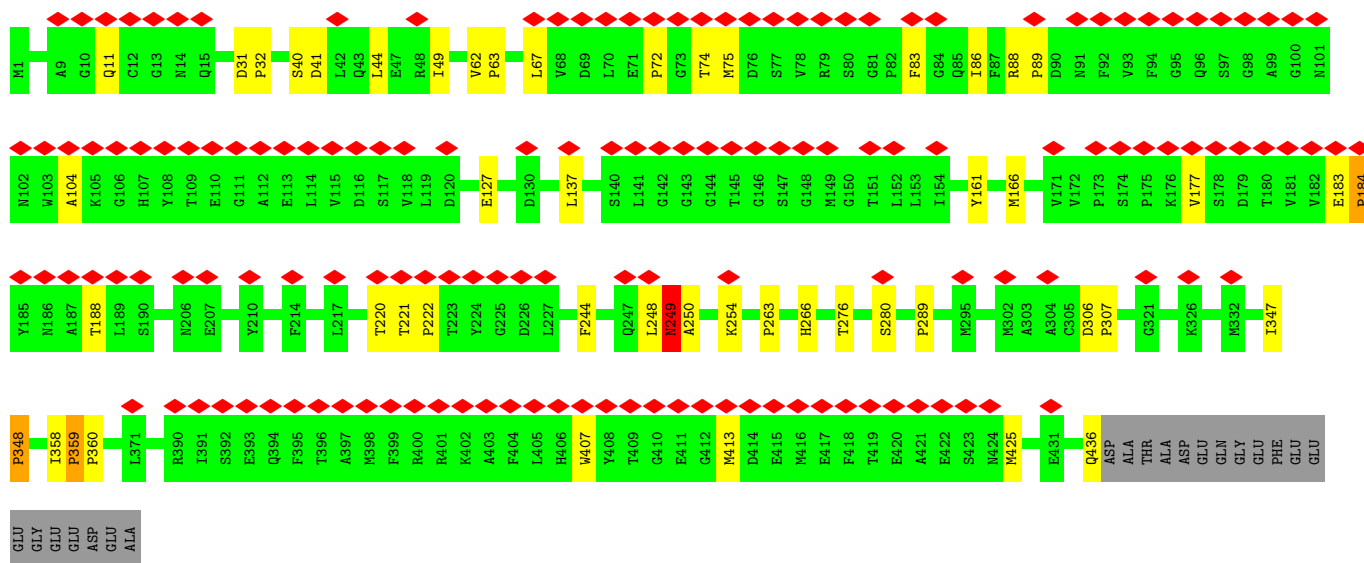
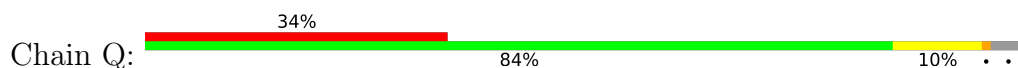


- Molecule 2: Tubulin beta chain

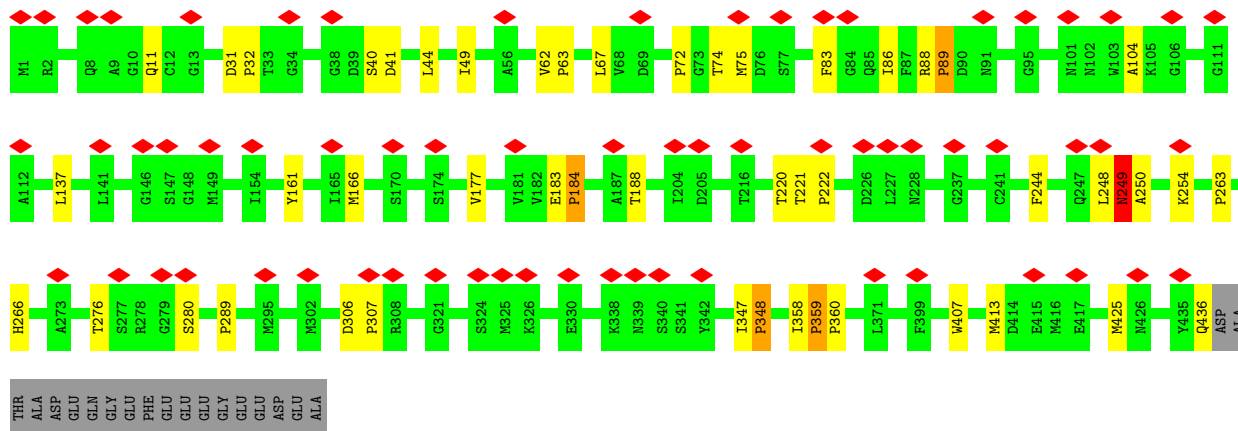
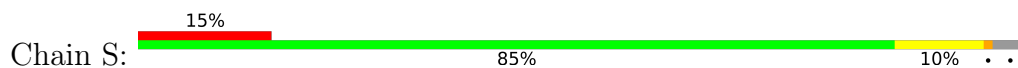




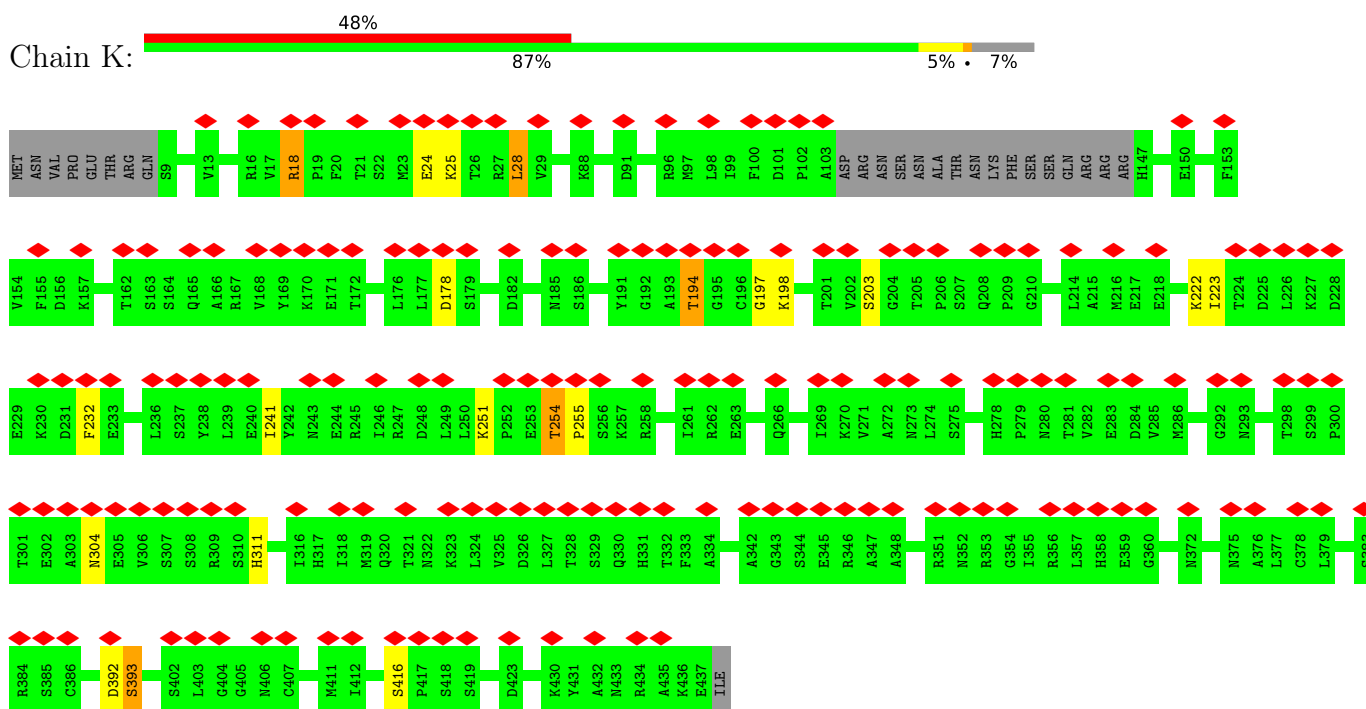
• Molecule 2: Tubulin beta chain



• Molecule 2: Tubulin beta chain



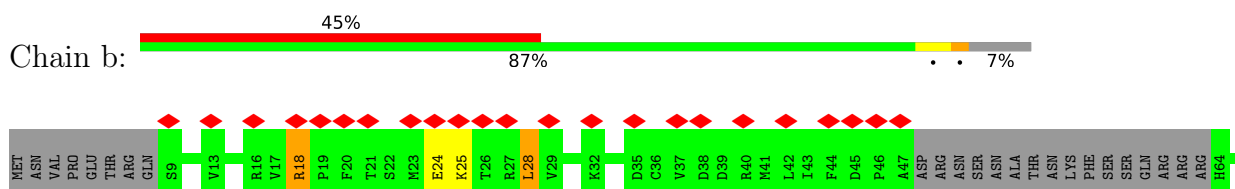
• Molecule 3: kinesin-8/ Kip3

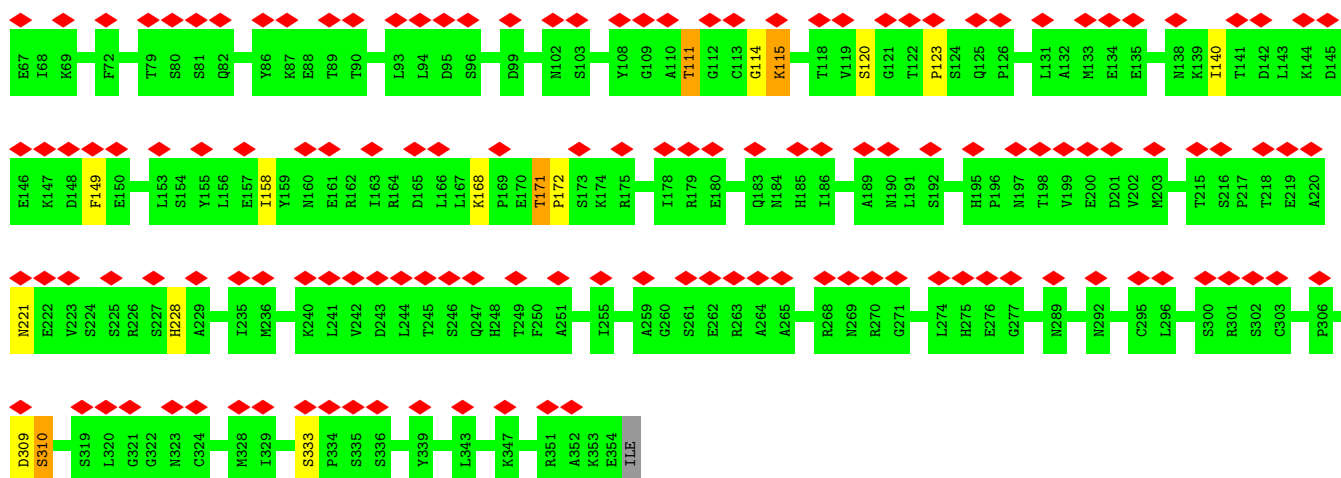


- Molecule 3: kinesin-8/ Kip3

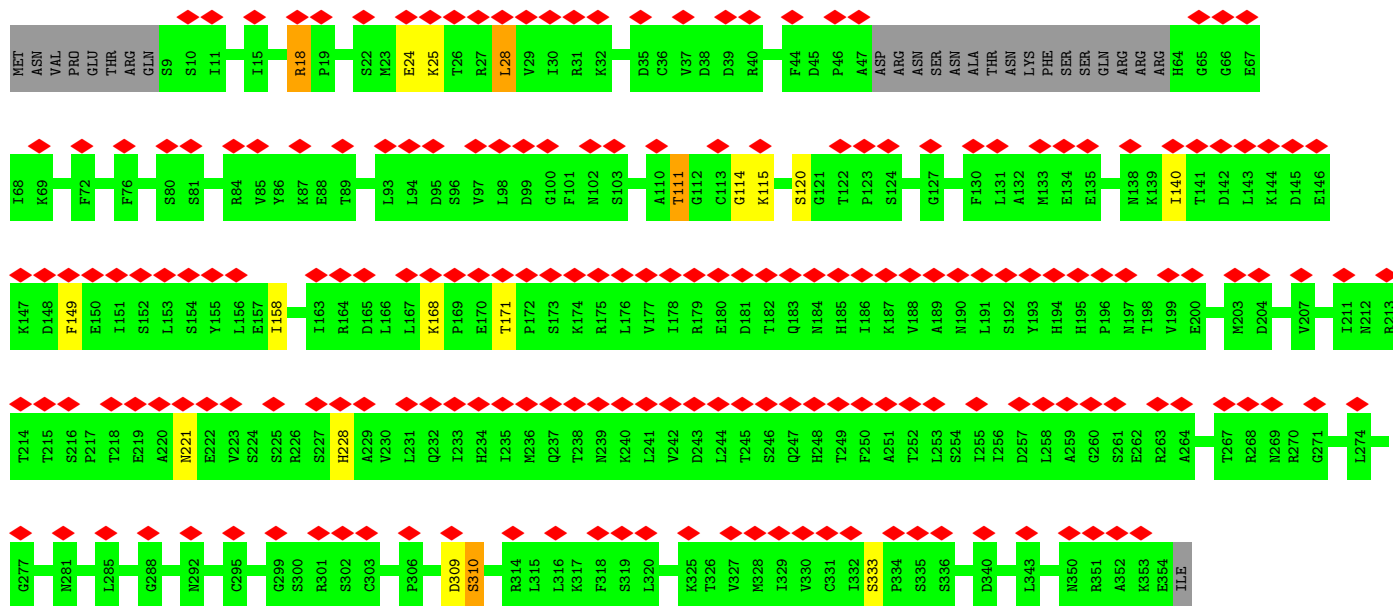
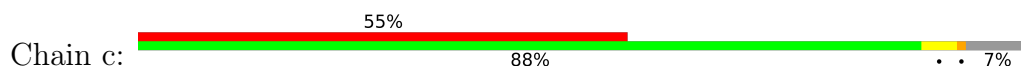


- Molecule 3: kinesin-8/ Kip3

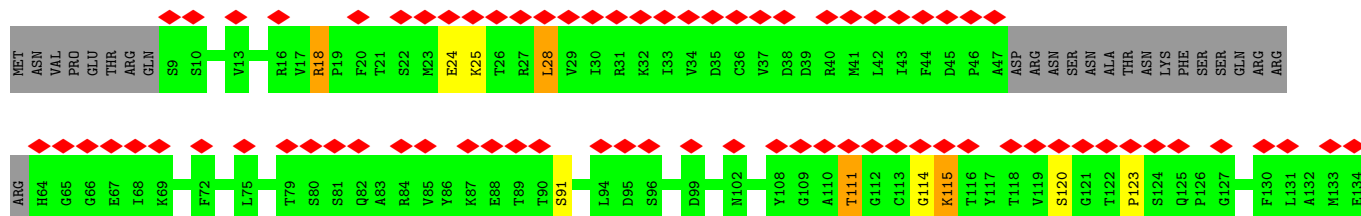
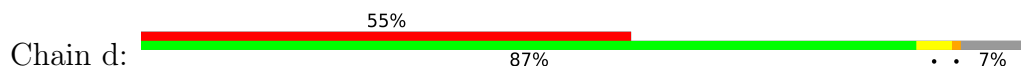


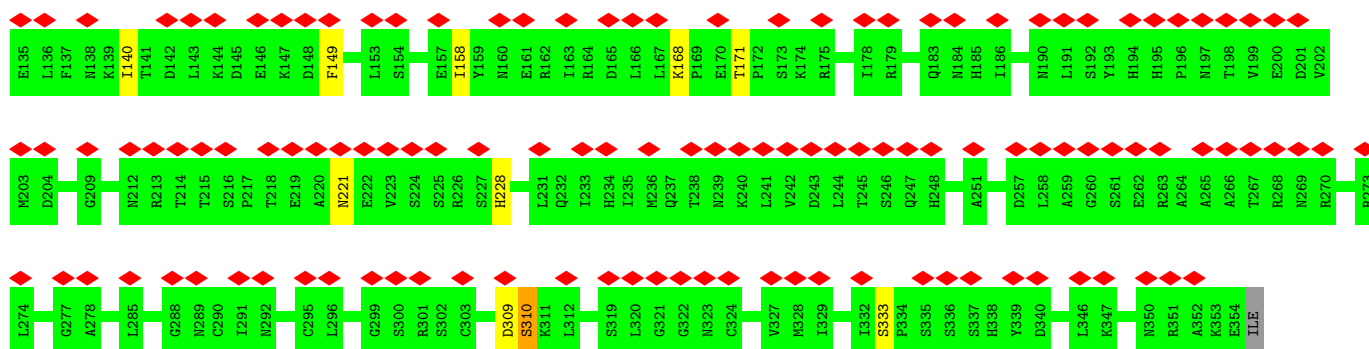


• Molecule 3: kinesin-8/ Kip3

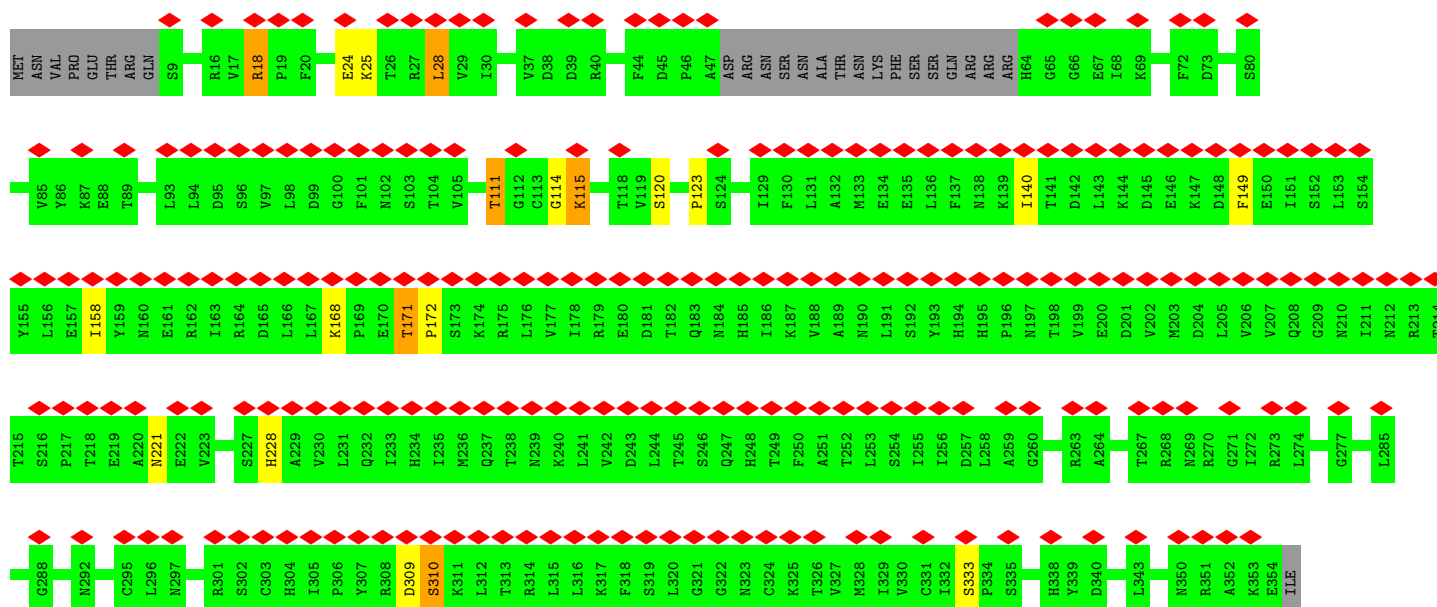
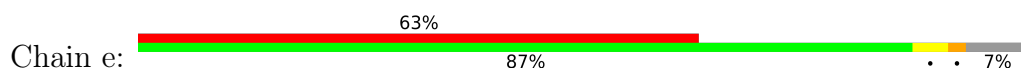


• Molecule 3: kinesin-8/ Kip3

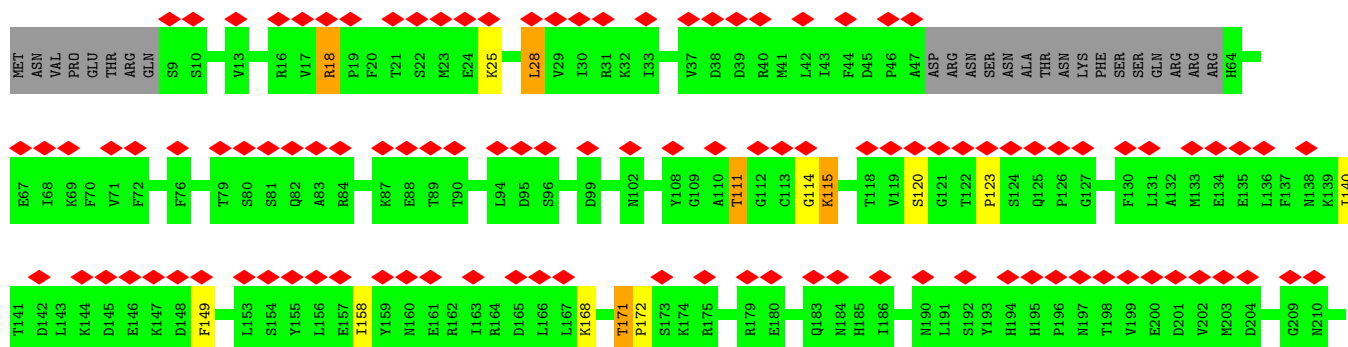
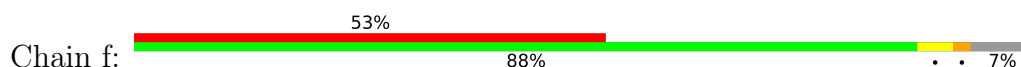


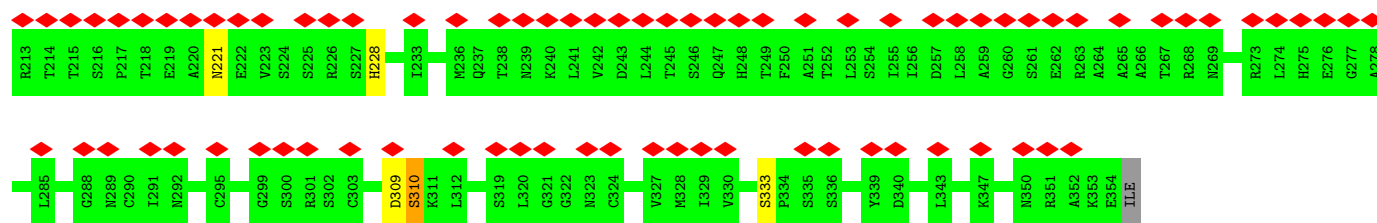


• Molecule 3: kinesin-8/ Kip3

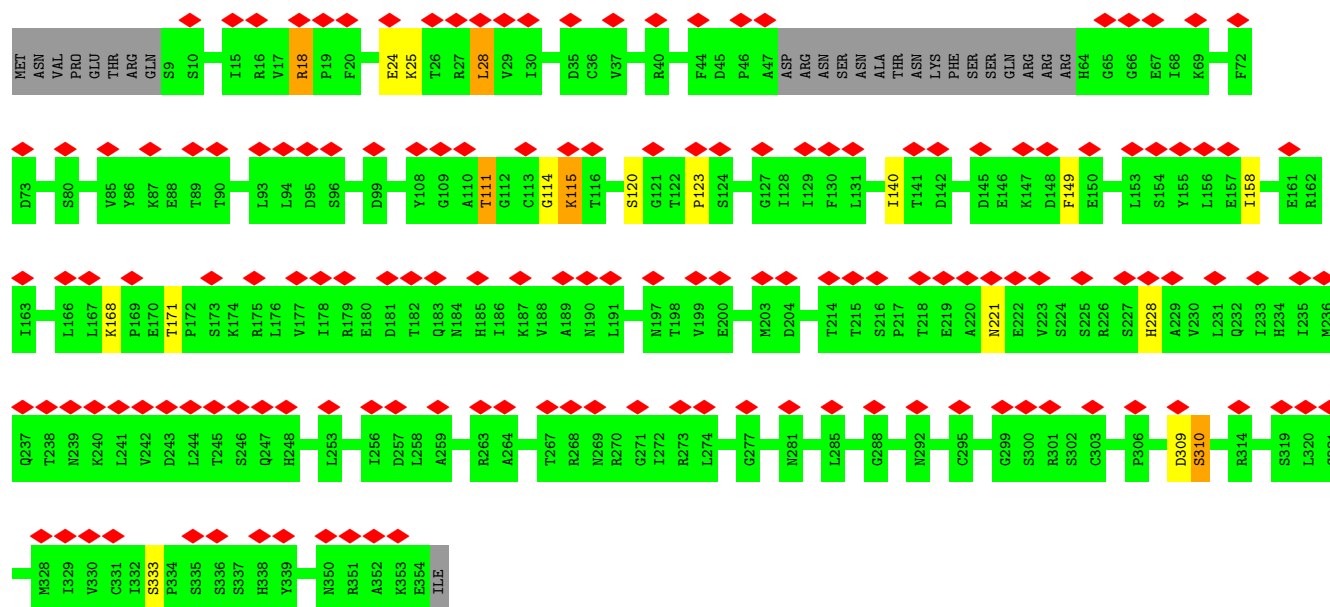
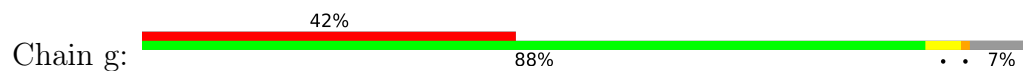


• Molecule 3: kinesin-8/ Kip3

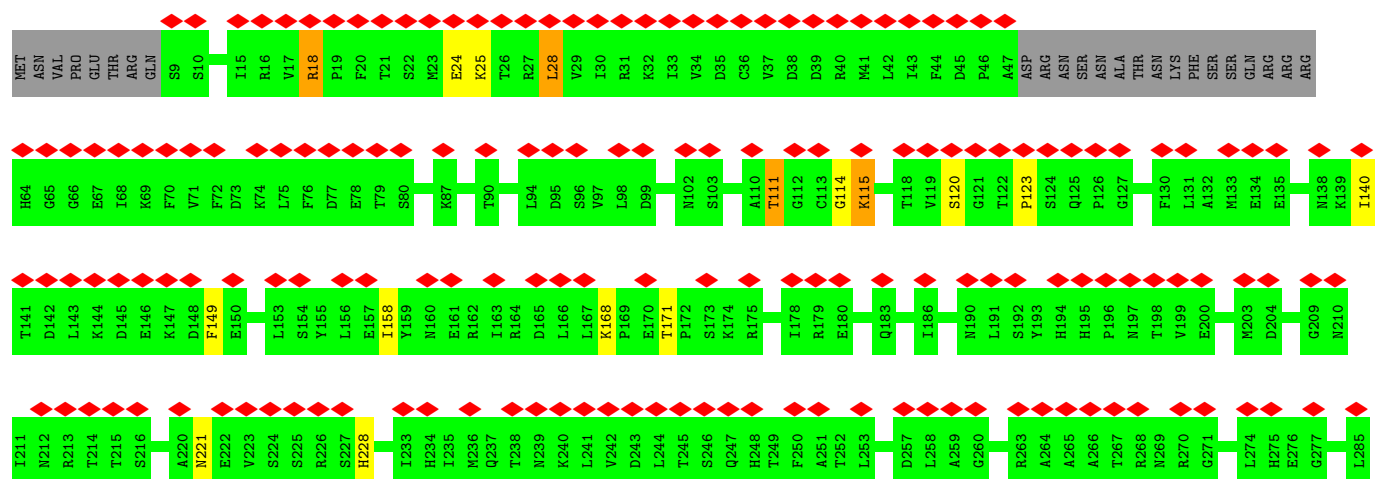
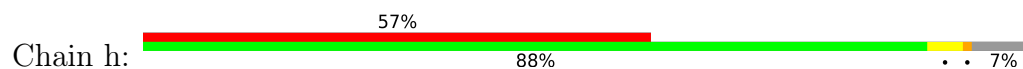


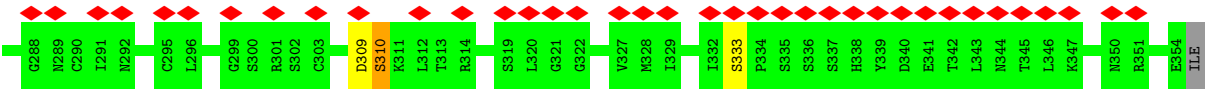


• Molecule 3: kinesin-8/ Kip3



• Molecule 3: kinesin-8/ Kip3





4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=-25.76°, rise=8.90 Å, axial sym=C14	Depositor
Number of segments used	21788	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; The contrast transfer function (CTF) was estimated using CTFFIND4 [(Rohou and Grigorieff, 2015) CTFFIND4: Fast and accurate] with a 500 um step search. A second CTFFIND run with a 100 um step search was carried out to refine the initial defocus values. Micrographs whose estimated resolution was lower than 8 Angstrom with 0.8 confidence were excluded.	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	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	14.475	Depositor
Minimum map value	-10.953	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.366	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	294.0, 294.0, 294.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.98, 0.98, 0.98	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: MG, GTP, G2P, ANP

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	0.65	0/3435	0.85	14/4663 (0.3%)
1	C	0.65	0/3435	0.85	14/4663 (0.3%)
1	E	0.65	0/3435	0.85	12/4663 (0.3%)
1	G	0.65	0/3435	0.85	12/4663 (0.3%)
1	I	0.65	0/3435	0.85	12/4663 (0.3%)
1	L	0.65	0/3435	0.85	12/4663 (0.3%)
1	N	0.65	0/3435	0.85	12/4663 (0.3%)
1	P	0.65	0/3435	0.85	12/4663 (0.3%)
1	R	0.65	0/3435	0.85	12/4663 (0.3%)
2	B	0.65	0/3426	0.83	10/4641 (0.2%)
2	D	0.65	0/3426	0.83	10/4641 (0.2%)
2	F	0.65	0/3426	0.83	10/4641 (0.2%)
2	H	0.65	0/3426	0.83	10/4641 (0.2%)
2	J	0.65	0/3426	0.83	10/4641 (0.2%)
2	M	0.65	0/3426	0.83	10/4641 (0.2%)
2	O	0.65	0/3426	0.83	10/4641 (0.2%)
2	Q	0.65	0/3426	0.83	10/4641 (0.2%)
2	S	0.65	0/3426	0.83	10/4641 (0.2%)
3	K	0.64	0/2625	0.85	8/3550 (0.2%)
3	a	0.64	0/2625	0.85	8/3550 (0.2%)
3	b	0.64	0/2625	0.85	8/3550 (0.2%)
3	c	0.64	0/2625	0.85	8/3550 (0.2%)
3	d	0.64	0/2625	0.85	10/3550 (0.3%)
3	e	0.64	0/2625	0.85	8/3550 (0.2%)
3	f	0.64	0/2625	0.85	8/3550 (0.2%)
3	g	0.64	0/2625	0.85	8/3550 (0.2%)
3	h	0.64	0/2625	0.85	8/3550 (0.2%)
All	All	0.65	0/85374	0.84	276/115686 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	E	0	1
1	G	0	1
1	I	0	1
1	L	0	1
1	N	0	1
1	P	0	1
1	R	0	1
2	B	0	1
2	D	0	1
2	F	0	1
2	H	0	1
2	J	0	1
2	M	0	1
2	O	0	1
2	Q	0	1
2	S	0	1
3	K	0	2
3	a	0	2
3	b	0	2
3	c	0	2
3	d	0	2
3	e	0	2
3	f	0	2
3	g	0	2
3	h	0	2
All	All	0	36

There are no bond length outliers.

All (276) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	359	PRO	CA-C-N	8.74	128.78	119.78
2	Q	359	PRO	C-N-CA	8.74	128.78	119.78
2	H	359	PRO	CA-C-N	8.70	128.74	119.78
2	H	359	PRO	C-N-CA	8.70	128.74	119.78
2	O	359	PRO	CA-C-N	8.70	128.74	119.78
2	O	359	PRO	C-N-CA	8.70	128.74	119.78
2	M	359	PRO	CA-C-N	8.67	128.71	119.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	359	PRO	C-N-CA	8.67	128.71	119.78
2	B	359	PRO	CA-C-N	8.64	128.68	119.78
2	B	359	PRO	C-N-CA	8.64	128.68	119.78
2	D	359	PRO	CA-C-N	8.64	128.68	119.78
2	D	359	PRO	C-N-CA	8.64	128.68	119.78
2	S	359	PRO	CA-C-N	8.64	128.68	119.78
2	S	359	PRO	C-N-CA	8.64	128.68	119.78
2	F	359	PRO	CA-C-N	8.64	128.68	119.78
2	F	359	PRO	C-N-CA	8.64	128.68	119.78
2	J	359	PRO	CA-C-N	8.62	128.66	119.78
2	J	359	PRO	C-N-CA	8.62	128.66	119.78
3	a	333	SER	CA-C-N	7.70	127.37	119.82
3	a	333	SER	C-N-CA	7.70	127.37	119.82
3	c	333	SER	CA-C-N	7.66	127.33	119.82
3	c	333	SER	C-N-CA	7.66	127.33	119.82
3	f	333	SER	CA-C-N	7.64	127.31	119.82
3	f	333	SER	C-N-CA	7.64	127.31	119.82
3	K	416	SER	CA-C-N	7.64	127.30	119.82
3	K	416	SER	C-N-CA	7.64	127.30	119.82
3	h	333	SER	CA-C-N	7.62	127.29	119.82
3	h	333	SER	C-N-CA	7.62	127.29	119.82
3	d	333	SER	CA-C-N	7.62	127.28	119.82
3	d	333	SER	C-N-CA	7.62	127.28	119.82
3	b	333	SER	CA-C-N	7.59	127.26	119.82
3	b	333	SER	C-N-CA	7.59	127.26	119.82
3	g	333	SER	CA-C-N	7.57	127.24	119.82
3	g	333	SER	C-N-CA	7.57	127.24	119.82
3	e	333	SER	CA-C-N	7.57	127.24	119.82
3	e	333	SER	C-N-CA	7.57	127.24	119.82
1	G	359	PRO	CA-C-N	7.10	128.72	119.84
1	G	359	PRO	C-N-CA	7.10	128.72	119.84
1	E	359	PRO	CA-C-N	7.05	128.66	119.84
1	E	359	PRO	C-N-CA	7.05	128.66	119.84
1	R	359	PRO	CA-C-N	7.05	128.65	119.84
1	R	359	PRO	C-N-CA	7.05	128.65	119.84
1	C	359	PRO	CA-C-N	7.04	128.65	119.84
1	C	359	PRO	C-N-CA	7.04	128.65	119.84
1	P	359	PRO	CA-C-N	7.04	128.65	119.84
1	P	359	PRO	C-N-CA	7.04	128.65	119.84
1	N	359	PRO	CA-C-N	7.04	128.64	119.84
1	N	359	PRO	C-N-CA	7.04	128.64	119.84
1	A	359	PRO	CA-C-N	7.03	128.63	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	359	PRO	C-N-CA	7.03	128.63	119.84
1	I	359	PRO	CA-C-N	7.03	128.63	119.84
1	I	359	PRO	C-N-CA	7.03	128.63	119.84
1	L	359	PRO	CA-C-N	7.02	128.62	119.84
1	L	359	PRO	C-N-CA	7.02	128.62	119.84
1	R	183	GLU	CA-C-N	6.68	126.47	119.05
1	R	183	GLU	C-N-CA	6.68	126.47	119.05
1	A	183	GLU	CA-C-N	6.63	126.41	119.05
1	A	183	GLU	C-N-CA	6.63	126.41	119.05
1	N	183	GLU	CA-C-N	6.62	126.40	119.05
1	N	183	GLU	C-N-CA	6.62	126.40	119.05
1	E	183	GLU	CA-C-N	6.61	126.39	119.05
1	E	183	GLU	C-N-CA	6.61	126.39	119.05
1	G	183	GLU	CA-C-N	6.61	126.39	119.05
1	G	183	GLU	C-N-CA	6.61	126.39	119.05
1	P	183	GLU	CA-C-N	6.61	126.38	119.05
1	P	183	GLU	C-N-CA	6.61	126.38	119.05
1	L	183	GLU	CA-C-N	6.60	126.37	119.05
1	L	183	GLU	C-N-CA	6.60	126.37	119.05
1	C	183	GLU	CA-C-N	6.59	126.36	119.05
1	C	183	GLU	C-N-CA	6.59	126.36	119.05
1	I	183	GLU	CA-C-N	6.58	126.36	119.05
1	I	183	GLU	C-N-CA	6.58	126.36	119.05
3	c	168	LYS	CA-C-N	6.46	126.59	119.87
3	c	168	LYS	C-N-CA	6.46	126.59	119.87
3	g	168	LYS	CA-C-N	6.46	126.58	119.87
3	g	168	LYS	C-N-CA	6.46	126.58	119.87
3	b	168	LYS	CA-C-N	6.45	126.58	119.87
3	b	168	LYS	C-N-CA	6.45	126.58	119.87
3	a	168	LYS	CA-C-N	6.44	126.57	119.87
3	a	168	LYS	C-N-CA	6.44	126.57	119.87
3	f	168	LYS	CA-C-N	6.44	126.56	119.87
3	f	168	LYS	C-N-CA	6.44	126.56	119.87
3	K	251	LYS	CA-C-N	6.43	126.56	119.87
3	K	251	LYS	C-N-CA	6.43	126.56	119.87
3	h	168	LYS	CA-C-N	6.43	126.56	119.87
3	h	168	LYS	C-N-CA	6.43	126.56	119.87
3	d	168	LYS	CA-C-N	6.37	126.50	119.87
3	d	168	LYS	C-N-CA	6.37	126.50	119.87
3	e	168	LYS	CA-C-N	6.36	126.48	119.87
3	e	168	LYS	C-N-CA	6.36	126.48	119.87
1	A	347	CYS	CA-C-N	6.14	125.83	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	347	CYS	C-N-CA	6.14	125.83	119.56
1	C	347	CYS	CA-C-N	6.10	125.79	119.56
1	C	347	CYS	C-N-CA	6.10	125.79	119.56
1	A	262	TYR	CA-C-N	6.04	127.39	119.84
1	A	262	TYR	C-N-CA	6.04	127.39	119.84
1	L	262	TYR	CA-C-N	6.03	127.38	119.84
1	L	262	TYR	C-N-CA	6.03	127.38	119.84
1	C	262	TYR	CA-C-N	6.01	127.36	119.84
1	C	262	TYR	C-N-CA	6.01	127.36	119.84
1	E	262	TYR	CA-C-N	6.00	127.34	119.84
1	E	262	TYR	C-N-CA	6.00	127.34	119.84
1	G	262	TYR	CA-C-N	5.99	127.32	119.84
1	G	262	TYR	C-N-CA	5.99	127.32	119.84
1	P	262	TYR	CA-C-N	5.96	127.28	119.84
1	P	262	TYR	C-N-CA	5.96	127.28	119.84
1	R	262	TYR	CA-C-N	5.95	127.28	119.84
1	R	262	TYR	C-N-CA	5.95	127.28	119.84
1	I	262	TYR	CA-C-N	5.95	127.28	119.84
1	I	262	TYR	C-N-CA	5.95	127.28	119.84
1	N	262	TYR	CA-C-N	5.95	127.27	119.84
1	N	262	TYR	C-N-CA	5.95	127.27	119.84
3	f	171	THR	CA-C-N	5.94	127.27	119.84
3	f	171	THR	C-N-CA	5.94	127.27	119.84
3	e	171	THR	CA-C-N	5.94	127.26	119.84
3	e	171	THR	C-N-CA	5.94	127.26	119.84
3	K	254	THR	CA-C-N	5.93	127.25	119.84
3	K	254	THR	C-N-CA	5.93	127.25	119.84
3	a	171	THR	CA-C-N	5.93	127.25	119.84
3	a	171	THR	C-N-CA	5.93	127.25	119.84
3	c	171	THR	CA-C-N	5.92	127.24	119.84
3	c	171	THR	C-N-CA	5.92	127.24	119.84
3	d	171	THR	CA-C-N	5.91	127.23	119.84
3	d	171	THR	C-N-CA	5.91	127.23	119.84
3	g	171	THR	CA-C-N	5.91	127.23	119.84
3	g	171	THR	C-N-CA	5.91	127.23	119.84
3	b	171	THR	CA-C-N	5.90	127.22	119.84
3	b	171	THR	C-N-CA	5.90	127.22	119.84
3	h	171	THR	CA-C-N	5.89	127.21	119.84
3	h	171	THR	C-N-CA	5.89	127.21	119.84
2	H	161	TYR	CA-C-N	5.83	125.51	119.56
2	H	161	TYR	C-N-CA	5.83	125.51	119.56
2	S	161	TYR	CA-C-N	5.83	125.51	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	161	TYR	C-N-CA	5.83	125.51	119.56
2	B	161	TYR	CA-C-N	5.83	125.50	119.56
2	B	161	TYR	C-N-CA	5.83	125.50	119.56
1	P	62	VAL	CA-C-N	5.82	126.71	120.13
1	P	62	VAL	C-N-CA	5.82	126.71	120.13
2	F	161	TYR	CA-C-N	5.81	125.49	119.56
2	F	161	TYR	C-N-CA	5.81	125.49	119.56
2	O	161	TYR	CA-C-N	5.81	125.48	119.56
2	O	161	TYR	C-N-CA	5.81	125.48	119.56
2	M	161	TYR	CA-C-N	5.80	125.47	119.56
2	M	161	TYR	C-N-CA	5.80	125.47	119.56
1	N	62	VAL	CA-C-N	5.79	126.67	120.13
1	N	62	VAL	C-N-CA	5.79	126.67	120.13
1	R	62	VAL	CA-C-N	5.79	126.67	120.13
1	R	62	VAL	C-N-CA	5.79	126.67	120.13
1	G	62	VAL	CA-C-N	5.78	126.66	120.13
1	G	62	VAL	C-N-CA	5.78	126.66	120.13
2	J	161	TYR	CA-C-N	5.78	125.45	119.56
2	J	161	TYR	C-N-CA	5.78	125.45	119.56
2	Q	161	TYR	CA-C-N	5.77	125.44	119.56
2	Q	161	TYR	C-N-CA	5.77	125.44	119.56
2	D	161	TYR	CA-C-N	5.76	125.44	119.56
2	D	161	TYR	C-N-CA	5.76	125.44	119.56
1	I	62	VAL	CA-C-N	5.76	126.64	120.13
1	I	62	VAL	C-N-CA	5.76	126.64	120.13
1	L	62	VAL	CA-C-N	5.75	126.63	120.13
1	L	62	VAL	C-N-CA	5.75	126.63	120.13
1	A	62	VAL	CA-C-N	5.75	126.62	120.13
1	A	62	VAL	C-N-CA	5.75	126.62	120.13
1	C	62	VAL	CA-C-N	5.74	126.61	120.13
1	C	62	VAL	C-N-CA	5.74	126.61	120.13
1	E	62	VAL	CA-C-N	5.72	126.60	120.13
1	E	62	VAL	C-N-CA	5.72	126.60	120.13
1	G	324	VAL	CA-C-N	5.71	126.98	119.84
1	G	324	VAL	C-N-CA	5.71	126.98	119.84
1	P	324	VAL	CA-C-N	5.71	126.97	119.84
1	P	324	VAL	C-N-CA	5.71	126.97	119.84
1	A	324	VAL	CA-C-N	5.67	126.93	119.84
1	A	324	VAL	C-N-CA	5.67	126.93	119.84
1	N	324	VAL	CA-C-N	5.65	126.90	119.84
1	N	324	VAL	C-N-CA	5.65	126.90	119.84
1	L	324	VAL	CA-C-N	5.64	126.89	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	324	VAL	C-N-CA	5.64	126.89	119.84
1	C	324	VAL	CA-C-N	5.64	126.89	119.84
1	C	324	VAL	C-N-CA	5.64	126.89	119.84
1	E	324	VAL	CA-C-N	5.64	126.89	119.84
1	E	324	VAL	C-N-CA	5.64	126.89	119.84
1	R	324	VAL	CA-C-N	5.63	126.87	119.84
1	R	324	VAL	C-N-CA	5.63	126.87	119.84
1	I	324	VAL	CA-C-N	5.61	126.85	119.84
1	I	324	VAL	C-N-CA	5.61	126.85	119.84
3	d	18	ARG	CA-C-N	5.61	126.39	120.11
3	d	18	ARG	C-N-CA	5.61	126.39	120.11
3	K	18	ARG	CA-C-N	5.61	126.39	120.11
3	K	18	ARG	C-N-CA	5.61	126.39	120.11
3	f	18	ARG	CA-C-N	5.61	126.39	120.11
3	f	18	ARG	C-N-CA	5.61	126.39	120.11
3	h	18	ARG	CA-C-N	5.60	126.38	120.11
3	h	18	ARG	C-N-CA	5.60	126.38	120.11
3	e	18	ARG	CA-C-N	5.57	126.35	120.11
3	e	18	ARG	C-N-CA	5.57	126.35	120.11
3	g	18	ARG	CA-C-N	5.56	126.34	120.11
3	g	18	ARG	C-N-CA	5.56	126.34	120.11
3	b	18	ARG	CA-C-N	5.56	126.34	120.11
3	b	18	ARG	C-N-CA	5.56	126.34	120.11
3	a	18	ARG	CA-C-N	5.54	126.32	120.11
3	a	18	ARG	C-N-CA	5.54	126.32	120.11
3	c	18	ARG	CA-C-N	5.54	126.31	120.11
3	c	18	ARG	C-N-CA	5.54	126.31	120.11
1	L	306	ASP	CA-C-N	5.43	126.63	119.84
1	L	306	ASP	C-N-CA	5.43	126.63	119.84
1	P	306	ASP	CA-C-N	5.41	126.60	119.84
1	P	306	ASP	C-N-CA	5.41	126.60	119.84
2	M	244	PHE	CA-C-N	5.41	126.55	120.66
2	M	244	PHE	C-N-CA	5.41	126.55	120.66
2	B	244	PHE	CA-C-N	5.40	126.55	120.66
2	B	244	PHE	C-N-CA	5.40	126.55	120.66
1	G	306	ASP	CA-C-N	5.39	126.58	119.84
1	G	306	ASP	C-N-CA	5.39	126.58	119.84
2	Q	244	PHE	CA-C-N	5.39	126.53	120.66
2	Q	244	PHE	C-N-CA	5.39	126.53	120.66
2	J	244	PHE	CA-C-N	5.38	126.53	120.66
2	J	244	PHE	C-N-CA	5.38	126.53	120.66
1	A	306	ASP	CA-C-N	5.38	126.56	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	306	ASP	C-N-CA	5.38	126.56	119.84
1	E	306	ASP	CA-C-N	5.38	126.56	119.84
1	E	306	ASP	C-N-CA	5.38	126.56	119.84
1	N	306	ASP	CA-C-N	5.38	126.56	119.84
1	N	306	ASP	C-N-CA	5.38	126.56	119.84
1	R	306	ASP	CA-C-N	5.38	126.56	119.84
1	R	306	ASP	C-N-CA	5.38	126.56	119.84
1	C	306	ASP	CA-C-N	5.37	126.55	119.84
1	C	306	ASP	C-N-CA	5.37	126.55	119.84
1	I	306	ASP	CA-C-N	5.37	126.55	119.84
1	I	306	ASP	C-N-CA	5.37	126.55	119.84
2	H	244	PHE	CA-C-N	5.37	126.51	120.66
2	H	244	PHE	C-N-CA	5.37	126.51	120.66
2	S	244	PHE	CA-C-N	5.37	126.51	120.66
2	S	244	PHE	C-N-CA	5.37	126.51	120.66
2	M	358	ILE	CA-C-N	5.36	125.90	120.38
2	M	358	ILE	C-N-CA	5.36	125.90	120.38
2	O	244	PHE	CA-C-N	5.35	126.50	120.66
2	O	244	PHE	C-N-CA	5.35	126.50	120.66
2	H	358	ILE	CA-C-N	5.33	125.87	120.38
2	H	358	ILE	C-N-CA	5.33	125.87	120.38
2	F	244	PHE	CA-C-N	5.33	126.47	120.66
2	F	244	PHE	C-N-CA	5.33	126.47	120.66
2	D	244	PHE	CA-C-N	5.32	126.46	120.66
2	D	244	PHE	C-N-CA	5.32	126.46	120.66
2	F	358	ILE	CA-C-N	5.32	125.86	120.38
2	F	358	ILE	C-N-CA	5.32	125.86	120.38
2	H	306	ASP	CA-C-N	5.30	126.47	119.84
2	H	306	ASP	C-N-CA	5.30	126.47	119.84
2	J	358	ILE	CA-C-N	5.30	125.84	120.38
2	J	358	ILE	C-N-CA	5.30	125.84	120.38
2	B	358	ILE	CA-C-N	5.29	125.83	120.38
2	B	358	ILE	C-N-CA	5.29	125.83	120.38
2	D	306	ASP	CA-C-N	5.28	126.44	119.84
2	D	306	ASP	C-N-CA	5.28	126.44	119.84
2	Q	358	ILE	CA-C-N	5.28	125.81	120.38
2	Q	358	ILE	C-N-CA	5.28	125.81	120.38
2	D	358	ILE	CA-C-N	5.27	125.81	120.38
2	D	358	ILE	C-N-CA	5.27	125.81	120.38
2	O	358	ILE	CA-C-N	5.26	125.80	120.38
2	O	358	ILE	C-N-CA	5.26	125.80	120.38
2	S	358	ILE	CA-C-N	5.25	125.79	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	358	ILE	C-N-CA	5.25	125.79	120.38
2	M	306	ASP	CA-C-N	5.22	126.36	119.84
2	M	306	ASP	C-N-CA	5.22	126.36	119.84
2	O	306	ASP	CA-C-N	5.22	126.36	119.84
2	O	306	ASP	C-N-CA	5.22	126.36	119.84
2	S	306	ASP	CA-C-N	5.22	126.36	119.84
2	S	306	ASP	C-N-CA	5.22	126.36	119.84
2	J	306	ASP	CA-C-N	5.20	126.33	119.84
2	J	306	ASP	C-N-CA	5.20	126.33	119.84
2	F	306	ASP	CA-C-N	5.19	126.33	119.84
2	F	306	ASP	C-N-CA	5.19	126.33	119.84
2	B	306	ASP	CA-C-N	5.19	126.33	119.84
2	B	306	ASP	C-N-CA	5.19	126.33	119.84
2	Q	306	ASP	CA-C-N	5.19	126.33	119.84
2	Q	306	ASP	C-N-CA	5.19	126.33	119.84
3	d	91	SER	CA-C-N	5.01	124.50	119.19
3	d	91	SER	C-N-CA	5.01	124.50	119.19

There are no chirality outliers.

All (36) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	267	PHE	Peptide
2	B	249	ASN	Peptide
1	C	267	PHE	Peptide
2	D	249	ASN	Peptide
1	E	267	PHE	Peptide
2	F	249	ASN	Peptide
1	G	267	PHE	Peptide
2	H	249	ASN	Peptide
1	I	267	PHE	Peptide
2	J	249	ASN	Peptide
3	K	28	LEU	Peptide,Mainchain
1	L	267	PHE	Peptide
2	M	249	ASN	Peptide
1	N	267	PHE	Peptide
2	O	249	ASN	Peptide
1	P	267	PHE	Peptide
2	Q	249	ASN	Peptide
1	R	267	PHE	Peptide
2	S	249	ASN	Peptide
3	a	28	LEU	Peptide,Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
3	b	28	LEU	Peptide,Mainchain
3	c	28	LEU	Peptide,Mainchain
3	d	28	LEU	Peptide,Mainchain
3	e	28	LEU	Peptide,Mainchain
3	f	28	LEU	Peptide,Mainchain
3	g	28	LEU	Peptide,Mainchain
3	h	28	LEU	Peptide,Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3358	3276	3277	20	0
1	C	3358	3276	3277	20	0
1	E	3358	3276	3277	20	0
1	G	3358	3276	3277	25	0
1	I	3358	3276	3277	26	0
1	L	3358	3276	3277	20	0
1	N	3358	3276	3277	21	0
1	P	3358	3276	3277	24	0
1	R	3358	3276	3277	26	0
2	B	3351	3235	3237	25	0
2	D	3351	3235	3237	25	0
2	F	3351	3235	3237	26	0
2	H	3351	3235	3237	36	0
2	J	3351	3235	3237	28	0
2	M	3351	3235	3237	35	0
2	O	3351	3235	3237	26	0
2	Q	3351	3235	3237	27	0
2	S	3351	3235	3237	27	0
3	K	2585	2607	2603	14	0
3	a	2585	2607	2603	11	0
3	b	2585	2607	2603	12	0
3	c	2585	2607	2603	11	0
3	d	2585	2607	2603	12	0
3	e	2585	2607	2603	12	0
3	f	2585	2607	2603	12	0
3	g	2585	2607	2603	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	h	2585	2607	2603	11	0
4	A	32	12	12	0	0
4	C	32	12	12	0	0
4	E	32	12	12	0	0
4	G	32	12	12	0	0
4	I	32	12	12	0	0
4	L	32	12	12	0	0
4	N	32	12	12	0	0
4	P	32	12	12	0	0
4	R	32	12	12	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
5	M	1	0	0	0	0
5	N	1	0	0	0	0
5	O	1	0	0	0	0
5	P	1	0	0	0	0
5	Q	1	0	0	0	0
5	R	1	0	0	0	0
5	S	1	0	0	0	0
5	a	1	0	0	0	0
5	b	1	0	0	0	0
5	c	1	0	0	0	0
5	d	1	0	0	0	0
5	e	1	0	0	0	0
5	f	1	0	0	0	0
5	g	1	0	0	0	0
5	h	1	0	0	0	0
6	B	32	14	14	1	0
6	D	32	14	14	1	0
6	F	32	14	14	1	0
6	H	32	14	14	1	0
6	J	32	14	14	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	M	32	14	14	1	0
6	O	32	14	14	1	0
6	Q	32	14	14	1	0
6	S	32	14	14	1	0
7	K	31	13	13	3	0
7	a	31	13	13	2	0
7	b	31	13	13	2	0
7	c	31	13	13	3	0
7	d	31	13	13	3	0
7	e	31	13	13	2	0
7	f	31	13	13	3	0
7	g	31	13	13	2	0
7	h	31	13	13	2	0
All	All	84528	82413	82404	546	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 3.

All (546) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:60:LYS:NZ	2:M:282:GLN:OE1	2.26	0.69
1:G:285:GLN:NE2	1:P:55:GLU:O	2.30	0.65
1:L:267:PHE:O	1:L:267:PHE:CD1	2.51	0.64
1:E:267:PHE:O	1:E:267:PHE:CD1	2.51	0.64
1:L:107:HIS:HD2	1:L:107:HIS:O	1.81	0.64
1:E:107:HIS:HD2	1:E:107:HIS:O	1.81	0.64
1:N:267:PHE:O	1:N:267:PHE:CD1	2.51	0.64
1:C:107:HIS:HD2	1:C:107:HIS:O	1.81	0.63
1:N:107:HIS:HD2	1:N:107:HIS:O	1.81	0.63
1:P:107:HIS:HD2	1:P:107:HIS:O	1.81	0.63
1:R:107:HIS:HD2	1:R:107:HIS:O	1.81	0.63
1:R:267:PHE:CD1	1:R:267:PHE:O	2.51	0.63
1:C:267:PHE:O	1:C:267:PHE:CD1	2.51	0.63
1:P:267:PHE:O	1:P:267:PHE:CD1	2.51	0.63
1:G:267:PHE:O	1:G:267:PHE:CD1	2.51	0.63
1:A:267:PHE:CD1	1:A:267:PHE:O	2.51	0.63
1:I:267:PHE:O	1:I:267:PHE:CD1	2.51	0.63
1:A:107:HIS:HD2	1:A:107:HIS:O	1.81	0.62
1:I:107:HIS:HD2	1:I:107:HIS:O	1.81	0.62
1:G:107:HIS:HD2	1:G:107:HIS:O	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:a:114:GLY:HA2	7:a:501:ANP:O2A	2.00	0.61
3:h:114:GLY:HA2	7:h:501:ANP:O2A	2.00	0.61
3:c:114:GLY:HA2	7:c:501:ANP:O2A	2.00	0.61
3:d:114:GLY:HA2	7:d:501:ANP:O2A	2.00	0.61
3:K:197:GLY:HA2	7:K:501:ANP:O2A	2.00	0.61
3:g:114:GLY:HA2	7:g:501:ANP:O2A	2.00	0.61
3:f:114:GLY:HA2	7:f:501:ANP:O2A	2.00	0.60
1:I:283:HIS:CB	1:R:88:HIS:HB3	2.32	0.60
3:b:114:GLY:HA2	7:b:501:ANP:O2A	2.00	0.60
3:e:114:GLY:HA2	7:e:501:ANP:O2A	2.00	0.60
3:d:115:LYS:HB2	3:d:115:LYS:NZ	2.18	0.59
3:g:115:LYS:HB2	3:g:115:LYS:NZ	2.18	0.59
3:K:198:LYS:HB2	3:K:198:LYS:NZ	2.18	0.59
3:c:115:LYS:HB2	3:c:115:LYS:NZ	2.18	0.59
3:b:115:LYS:HB2	3:b:115:LYS:NZ	2.18	0.59
3:h:115:LYS:HB2	3:h:115:LYS:NZ	2.18	0.59
3:a:115:LYS:HB2	3:a:115:LYS:NZ	2.18	0.58
3:e:115:LYS:NZ	3:e:115:LYS:HB2	2.18	0.58
3:f:115:LYS:HB2	3:f:115:LYS:NZ	2.18	0.58
2:F:248:LEU:N	2:F:248:LEU:HD23	2.20	0.57
2:M:248:LEU:N	2:M:248:LEU:HD23	2.20	0.57
2:O:248:LEU:HD23	2:O:248:LEU:N	2.20	0.57
2:B:248:LEU:N	2:B:248:LEU:HD23	2.20	0.56
2:H:248:LEU:N	2:H:248:LEU:HD23	2.20	0.56
2:J:248:LEU:HD23	2:J:248:LEU:N	2.20	0.56
1:I:88:HIS:HB3	1:N:283:HIS:CG	2.41	0.56
2:Q:248:LEU:HD23	2:Q:248:LEU:N	2.20	0.56
2:D:248:LEU:N	2:D:248:LEU:HD23	2.20	0.56
2:S:248:LEU:N	2:S:248:LEU:HD23	2.20	0.56
1:G:103:TYR:C	1:G:103:TYR:CD2	2.85	0.54
1:I:103:TYR:C	1:I:103:TYR:CD2	2.85	0.54
1:C:103:TYR:C	1:C:103:TYR:CD2	2.85	0.54
1:R:103:TYR:C	1:R:103:TYR:CD2	2.85	0.54
1:P:103:TYR:C	1:P:103:TYR:CD2	2.85	0.54
1:A:103:TYR:C	1:A:103:TYR:CD2	2.85	0.54
1:E:103:TYR:C	1:E:103:TYR:CD2	2.85	0.54
2:J:248:LEU:O	2:J:249:ASN:HB2	2.08	0.54
1:L:103:TYR:CD2	1:L:103:TYR:C	2.85	0.54
2:O:248:LEU:O	2:O:249:ASN:HB2	2.08	0.54
1:I:283:HIS:CG	1:R:88:HIS:HB3	2.42	0.54
2:B:248:LEU:O	2:B:249:ASN:HB2	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:248:LEU:O	2:F:249:ASN:HB2	2.08	0.54
2:M:248:LEU:O	2:M:249:ASN:HB2	2.08	0.54
1:N:103:TYR:C	1:N:103:TYR:CD2	2.85	0.54
2:H:248:LEU:O	2:H:249:ASN:HB2	2.08	0.53
3:a:309:ASP:O	3:a:310:SER:CB	2.56	0.53
1:E:107:HIS:O	1:E:107:HIS:CD2	2.61	0.53
2:H:127:GLU:OE1	2:M:338:LYS:NZ	2.39	0.53
1:I:283:HIS:HB3	1:R:88:HIS:HB3	1.90	0.53
3:e:309:ASP:O	3:e:310:SER:CB	2.56	0.53
1:N:107:HIS:O	1:N:107:HIS:CD2	2.61	0.53
2:S:248:LEU:O	2:S:249:ASN:HB2	2.08	0.53
2:D:248:LEU:O	2:D:249:ASN:HB2	2.08	0.53
1:L:107:HIS:O	1:L:107:HIS:CD2	2.61	0.53
3:h:309:ASP:O	3:h:310:SER:CB	2.56	0.53
3:g:309:ASP:O	3:g:310:SER:CB	2.56	0.53
3:b:309:ASP:O	3:b:310:SER:CB	2.56	0.53
2:Q:248:LEU:O	2:Q:249:ASN:HB2	2.08	0.53
1:I:285:GLN:NE2	1:R:55:GLU:O	2.42	0.53
2:M:266:HIS:CD2	2:M:266:HIS:O	2.62	0.53
3:f:309:ASP:O	3:f:310:SER:CB	2.56	0.53
2:F:266:HIS:CD2	2:F:266:HIS:O	2.62	0.53
1:I:227:LEU:C	1:I:227:LEU:HD23	2.34	0.53
2:O:266:HIS:CD2	2:O:266:HIS:O	2.62	0.53
1:G:227:LEU:C	1:G:227:LEU:HD23	2.34	0.53
2:S:266:HIS:O	2:S:266:HIS:CD2	2.62	0.53
2:B:266:HIS:O	2:B:266:HIS:CD2	2.62	0.52
1:I:107:HIS:O	1:I:107:HIS:CD2	2.61	0.52
1:L:227:LEU:C	1:L:227:LEU:HD23	2.34	0.52
1:R:227:LEU:C	1:R:227:LEU:HD23	2.34	0.52
1:C:227:LEU:C	1:C:227:LEU:HD23	2.34	0.52
2:D:266:HIS:O	2:D:266:HIS:CD2	2.62	0.52
1:N:227:LEU:C	1:N:227:LEU:HD23	2.34	0.52
2:Q:266:HIS:O	2:Q:266:HIS:CD2	2.62	0.52
2:S:436:GLN:O	2:S:436:GLN:HG2	2.10	0.52
1:A:227:LEU:C	1:A:227:LEU:HD23	2.34	0.52
2:D:436:GLN:O	2:D:436:GLN:HG2	2.10	0.52
1:E:227:LEU:HD23	1:E:227:LEU:C	2.34	0.52
2:Q:436:GLN:HG2	2:Q:436:GLN:O	2.10	0.52
2:B:436:GLN:HG2	2:B:436:GLN:O	2.10	0.52
2:H:266:HIS:CD2	2:H:266:HIS:O	2.62	0.52
2:J:266:HIS:O	2:J:266:HIS:CD2	2.62	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:436:GLN:O	2:J:436:GLN:HG2	2.10	0.52
1:P:227:LEU:C	1:P:227:LEU:HD23	2.34	0.52
3:K:392:ASP:O	3:K:393:SER:CB	2.56	0.52
1:G:107:HIS:O	1:G:107:HIS:CD2	2.61	0.52
2:H:436:GLN:O	2:H:436:GLN:HG2	2.10	0.52
2:O:248:LEU:O	2:O:249:ASN:CB	2.58	0.52
2:F:248:LEU:O	2:F:249:ASN:CB	2.58	0.52
3:d:309:ASP:O	3:d:310:SER:CB	2.56	0.52
2:M:104:ALA:HB2	2:M:413:MET:SD	2.50	0.52
2:M:248:LEU:O	2:M:249:ASN:CB	2.58	0.52
1:A:107:HIS:O	1:A:107:HIS:CD2	2.61	0.52
2:F:104:ALA:HB2	2:F:413:MET:SD	2.50	0.52
2:F:436:GLN:O	2:F:436:GLN:HG2	2.10	0.52
2:M:436:GLN:O	2:M:436:GLN:HG2	2.10	0.52
3:c:309:ASP:O	3:c:310:SER:CB	2.56	0.52
2:O:436:GLN:O	2:O:436:GLN:HG2	2.10	0.52
2:B:104:ALA:HB2	2:B:413:MET:SD	2.50	0.52
3:f:111:THR:OG1	3:f:221:ASN:ND2	2.43	0.52
2:S:104:ALA:HB2	2:S:413:MET:SD	2.50	0.52
2:H:104:ALA:HB2	2:H:413:MET:SD	2.50	0.52
1:I:267:PHE:CD1	1:I:267:PHE:C	2.86	0.52
2:O:104:ALA:HB2	2:O:413:MET:SD	2.50	0.52
1:A:267:PHE:CD1	1:A:267:PHE:C	2.86	0.51
3:K:198:LYS:HB2	3:K:198:LYS:HZ1	1.76	0.51
2:D:104:ALA:HB2	2:D:413:MET:SD	2.50	0.51
1:I:285:GLN:HB2	1:R:56:THR:HG22	1.92	0.51
2:J:104:ALA:HB2	2:J:413:MET:SD	2.50	0.51
3:g:115:LYS:HB2	3:g:115:LYS:HZ1	1.75	0.51
3:b:111:THR:OG1	3:b:221:ASN:ND2	2.43	0.51
3:e:111:THR:OG1	3:e:221:ASN:ND2	2.43	0.51
2:Q:104:ALA:HB2	2:Q:413:MET:SD	2.50	0.51
2:B:248:LEU:O	2:B:249:ASN:CB	2.58	0.51
3:K:194:THR:OG1	3:K:304:ASN:ND2	2.43	0.51
1:G:285:GLN:HB2	1:P:56:THR:HG22	1.92	0.51
3:g:111:THR:OG1	3:g:221:ASN:ND2	2.43	0.51
3:a:111:THR:OG1	3:a:221:ASN:ND2	2.43	0.51
1:E:267:PHE:CD1	1:E:267:PHE:C	2.86	0.51
2:F:276:THR:OG1	2:F:280:SER:OG	2.28	0.51
3:d:111:THR:OG1	3:d:221:ASN:ND2	2.43	0.51
1:L:267:PHE:CD1	1:L:267:PHE:C	2.86	0.51
2:M:276:THR:OG1	2:M:280:SER:OG	2.29	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:248:LEU:O	2:H:249:ASN:CB	2.58	0.51
3:h:111:THR:OG1	3:h:221:ASN:ND2	2.43	0.51
2:D:276:THR:OG1	2:D:280:SER:OG	2.29	0.51
3:c:111:THR:OG1	3:c:221:ASN:ND2	2.43	0.51
2:J:248:LEU:O	2:J:249:ASN:CB	2.58	0.51
1:N:267:PHE:CD1	1:N:267:PHE:C	2.86	0.51
2:S:276:THR:OG1	2:S:280:SER:OG	2.29	0.51
2:O:276:THR:OG1	2:O:280:SER:OG	2.29	0.51
2:Q:250:ALA:HA	2:Q:254:LYS:HD2	1.93	0.51
1:C:107:HIS:O	1:C:107:HIS:CD2	2.61	0.51
2:D:250:ALA:HA	2:D:254:LYS:HD2	1.93	0.51
1:P:107:HIS:O	1:P:107:HIS:CD2	2.61	0.51
2:Q:276:THR:OG1	2:Q:280:SER:OG	2.29	0.51
1:R:107:HIS:O	1:R:107:HIS:CD2	2.61	0.51
2:D:248:LEU:O	2:D:249:ASN:CB	2.58	0.51
2:H:276:THR:OG1	2:H:280:SER:OG	2.28	0.51
2:S:248:LEU:O	2:S:249:ASN:CB	2.58	0.51
2:S:250:ALA:HA	2:S:254:LYS:HD2	1.93	0.51
2:H:127:GLU:OE2	2:M:338:LYS:NZ	2.43	0.50
2:F:250:ALA:HA	2:F:254:LYS:HD2	1.93	0.50
2:O:250:ALA:HA	2:O:254:LYS:HD2	1.93	0.50
2:Q:248:LEU:O	2:Q:249:ASN:CB	2.58	0.50
2:B:250:ALA:HA	2:B:254:LYS:HD2	1.93	0.50
2:H:250:ALA:HA	2:H:254:LYS:HD2	1.93	0.50
1:I:183:GLU:HB2	1:I:184:PRO:HD3	1.93	0.50
3:d:115:LYS:HB2	3:d:115:LYS:HZ1	1.77	0.50
1:C:183:GLU:HB2	1:C:184:PRO:HD3	1.94	0.50
2:J:276:THR:OG1	2:J:280:SER:OG	2.29	0.50
1:P:183:GLU:HB2	1:P:184:PRO:HD3	1.94	0.50
1:R:183:GLU:HB2	1:R:184:PRO:HD3	1.94	0.50
2:B:276:THR:OG1	2:B:280:SER:OG	2.29	0.50
1:G:183:GLU:HB2	1:G:184:PRO:HD3	1.94	0.50
2:J:250:ALA:HA	2:J:254:LYS:HD2	1.93	0.50
1:A:183:GLU:HB2	1:A:184:PRO:HD3	1.94	0.50
1:G:267:PHE:CD1	1:G:267:PHE:C	2.86	0.50
2:M:250:ALA:HA	2:M:254:LYS:HD2	1.93	0.50
1:E:183:GLU:HB2	1:E:184:PRO:HD3	1.94	0.50
2:J:283:TYR:CD2	2:S:88:ARG:HA	2.47	0.50
1:L:183:GLU:HB2	1:L:184:PRO:HD3	1.94	0.50
1:N:183:GLU:HB2	1:N:184:PRO:HD3	1.94	0.50
1:N:177:VAL:HG12	1:N:177:VAL:O	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:177:VAL:HG12	1:R:177:VAL:O	2.11	0.49
1:C:177:VAL:HG12	1:C:177:VAL:O	2.11	0.49
1:G:183:GLU:N	1:G:184:PRO:CD	2.75	0.49
1:P:177:VAL:HG12	1:P:177:VAL:O	2.11	0.49
1:A:183:GLU:N	1:A:184:PRO:CD	2.75	0.49
1:A:358:GLN:O	1:A:358:GLN:HG3	2.13	0.49
1:E:177:VAL:HG12	1:E:177:VAL:O	2.11	0.49
1:I:183:GLU:N	1:I:184:PRO:CD	2.75	0.49
1:L:177:VAL:O	1:L:177:VAL:HG12	2.11	0.49
1:P:183:GLU:N	1:P:184:PRO:CD	2.75	0.49
1:C:183:GLU:N	1:C:184:PRO:CD	2.75	0.49
1:L:183:GLU:N	1:L:184:PRO:CD	2.75	0.49
1:N:183:GLU:N	1:N:184:PRO:CD	2.75	0.49
1:R:183:GLU:N	1:R:184:PRO:CD	2.75	0.49
1:E:183:GLU:N	1:E:184:PRO:CD	2.75	0.49
1:A:177:VAL:HG12	1:A:177:VAL:O	2.11	0.49
3:b:115:LYS:HB2	3:b:115:LYS:HZ1	1.78	0.49
1:G:358:GLN:HG3	1:G:358:GLN:O	2.13	0.49
3:f:115:LYS:HB2	3:f:115:LYS:HZ1	1.78	0.49
1:I:358:GLN:O	1:I:358:GLN:HG3	2.13	0.49
1:N:358:GLN:HG3	1:N:358:GLN:O	2.13	0.49
3:e:115:LYS:HB2	3:e:115:LYS:HZ1	1.78	0.49
1:E:358:GLN:HG3	1:E:358:GLN:O	2.13	0.48
1:L:358:GLN:HG3	1:L:358:GLN:O	2.13	0.48
2:H:85:GLN:HA	2:M:283:TYR:OH	2.13	0.48
1:I:177:VAL:HG12	1:I:177:VAL:O	2.11	0.48
2:M:11:GLN:HG2	2:M:74:THR:HG23	1.95	0.48
2:F:11:GLN:HG2	2:F:74:THR:HG23	1.94	0.48
2:O:11:GLN:HG2	2:O:74:THR:HG23	1.95	0.48
1:G:177:VAL:HG12	1:G:177:VAL:O	2.11	0.48
1:E:147:SER:OG	1:E:148:GLY:N	2.46	0.48
2:H:62:VAL:HG21	2:M:283:TYR:HA	1.94	0.48
1:L:147:SER:OG	1:L:148:GLY:N	2.46	0.48
1:N:147:SER:OG	1:N:148:GLY:N	2.46	0.48
2:B:11:GLN:HG2	2:B:74:THR:HG23	1.95	0.48
1:P:267:PHE:CD1	1:P:267:PHE:C	2.86	0.48
1:R:358:GLN:O	1:R:358:GLN:HG3	2.13	0.48
1:C:267:PHE:CD1	1:C:267:PHE:C	2.86	0.48
2:H:11:GLN:HG2	2:H:74:THR:HG23	1.94	0.48
1:C:358:GLN:O	1:C:358:GLN:HG3	2.13	0.48
2:J:11:GLN:HG2	2:J:74:THR:HG23	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:137:LEU:HB2	2:Q:166:MET:SD	2.54	0.48
1:R:267:PHE:CD1	1:R:267:PHE:C	2.86	0.48
2:S:137:LEU:HB2	2:S:166:MET:SD	2.54	0.48
1:A:147:SER:OG	1:A:148:GLY:N	2.46	0.48
2:D:11:GLN:HG2	2:D:74:THR:HG23	1.94	0.47
2:D:137:LEU:HB2	2:D:166:MET:SD	2.54	0.47
2:Q:11:GLN:HG2	2:Q:74:THR:HG23	1.94	0.47
2:H:283:TYR:CD2	2:Q:88:ARG:HA	2.49	0.47
1:P:358:GLN:O	1:P:358:GLN:HG3	2.13	0.47
2:S:11:GLN:HG2	2:S:74:THR:HG23	1.95	0.47
2:B:137:LEU:HB2	2:B:166:MET:SD	2.54	0.47
2:H:137:LEU:HB2	2:H:166:MET:SD	2.54	0.47
2:F:75:MET:HE2	2:F:75:MET:HA	1.96	0.47
2:J:137:LEU:HB2	2:J:166:MET:SD	2.54	0.47
2:D:183:GLU:HB2	2:D:184:PRO:HD3	1.96	0.47
2:F:137:LEU:HB2	2:F:166:MET:SD	2.54	0.47
2:H:57:ALA:CB	2:M:286:LEU:HG	2.45	0.47
2:H:183:GLU:HB2	2:H:184:PRO:HD3	1.96	0.47
2:M:75:MET:HE2	2:M:75:MET:HA	1.96	0.47
2:O:75:MET:HE2	2:O:75:MET:HA	1.96	0.47
2:S:183:GLU:HB2	2:S:184:PRO:HD3	1.96	0.47
2:B:75:MET:HA	2:B:75:MET:HE2	1.96	0.47
2:B:183:GLU:HB2	2:B:184:PRO:HD3	1.96	0.47
2:M:137:LEU:HB2	2:M:166:MET:SD	2.54	0.47
2:O:137:LEU:HB2	2:O:166:MET:SD	2.54	0.47
2:Q:183:GLU:HB2	2:Q:184:PRO:HD3	1.97	0.47
2:F:183:GLU:HB2	2:F:184:PRO:HD3	1.96	0.47
2:J:183:GLU:HB2	2:J:184:PRO:HD3	1.97	0.47
2:M:183:GLU:HB2	2:M:184:PRO:HD3	1.97	0.47
2:O:183:GLU:HB2	2:O:184:PRO:HD3	1.96	0.47
2:Q:75:MET:HE2	2:Q:75:MET:HA	1.96	0.46
2:H:75:MET:HE2	2:H:75:MET:HA	1.96	0.46
2:M:407:TRP:CE3	2:M:407:TRP:HA	2.50	0.46
2:F:407:TRP:CE3	2:F:407:TRP:HA	2.50	0.46
2:D:75:MET:HA	2:D:75:MET:HE2	1.96	0.46
1:G:283:HIS:HB3	1:P:88:HIS:HB3	1.97	0.46
2:H:57:ALA:H	2:M:285:ALA:HA	1.80	0.46
2:J:75:MET:HE2	2:J:75:MET:HA	1.96	0.46
2:S:407:TRP:HA	2:S:407:TRP:CE3	2.50	0.46
2:D:407:TRP:HA	2:D:407:TRP:CE3	2.50	0.46
2:H:407:TRP:HA	2:H:407:TRP:CE3	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:407:TRP:HA	2:O:407:TRP:CE3	2.50	0.46
2:S:75:MET:HA	2:S:75:MET:HE2	1.96	0.46
2:J:407:TRP:HA	2:J:407:TRP:CE3	2.50	0.46
2:Q:407:TRP:HA	2:Q:407:TRP:CE3	2.50	0.46
2:H:127:GLU:CD	2:M:338:LYS:NZ	2.73	0.46
2:B:407:TRP:HA	2:B:407:TRP:CE3	2.50	0.46
2:H:57:ALA:HB2	2:M:286:LEU:HG	1.98	0.45
3:a:140:ILE:HG23	3:a:149:PHE:CD1	2.52	0.45
3:h:140:ILE:HG23	3:h:149:PHE:CD1	2.52	0.45
1:I:367:ASP:O	1:I:368:LEU:C	2.59	0.45
3:g:140:ILE:HG23	3:g:149:PHE:CD1	2.52	0.45
1:C:367:ASP:O	1:C:368:LEU:C	2.59	0.45
1:G:367:ASP:O	1:G:368:LEU:C	2.59	0.45
2:H:338:LYS:NZ	2:Q:127:GLU:OE1	2.49	0.45
1:I:147:SER:OG	1:I:148:GLY:N	2.46	0.45
1:P:367:ASP:O	1:P:368:LEU:C	2.59	0.45
1:R:367:ASP:O	1:R:368:LEU:C	2.60	0.45
1:A:367:ASP:O	1:A:368:LEU:C	2.59	0.45
3:c:140:ILE:HG23	3:c:149:PHE:CD1	2.52	0.45
1:R:147:SER:OG	1:R:148:GLY:N	2.46	0.45
3:K:223:ILE:HG23	3:K:232:PHE:CD1	2.52	0.45
1:C:147:SER:OG	1:C:148:GLY:N	2.46	0.45
1:G:147:SER:OG	1:G:148:GLY:N	2.46	0.45
3:d:140:ILE:HG23	3:d:149:PHE:CD1	2.52	0.45
3:g:18:ARG:HD2	3:g:18:ARG:O	2.17	0.44
2:D:347:ILE:O	2:D:348:PRO:C	2.61	0.44
3:d:18:ARG:HD2	3:d:18:ARG:O	2.17	0.44
1:P:147:SER:OG	1:P:148:GLY:N	2.46	0.44
2:B:347:ILE:O	2:B:348:PRO:C	2.61	0.44
3:K:18:ARG:HD2	3:K:18:ARG:O	2.17	0.44
3:a:18:ARG:HD2	3:a:18:ARG:O	2.17	0.44
2:J:347:ILE:O	2:J:348:PRO:C	2.61	0.44
2:O:220:THR:OG1	2:O:221:THR:N	2.50	0.44
2:Q:347:ILE:O	2:Q:348:PRO:C	2.61	0.44
2:S:347:ILE:O	2:S:348:PRO:C	2.61	0.44
3:h:18:ARG:HD2	3:h:18:ARG:O	2.17	0.44
1:C:358:GLN:O	1:C:359:PRO:C	2.60	0.44
2:F:220:THR:OG1	2:F:221:THR:N	2.50	0.44
2:H:347:ILE:O	2:H:348:PRO:C	2.61	0.44
3:c:18:ARG:HD2	3:c:18:ARG:O	2.17	0.44
2:M:220:THR:OG1	2:M:221:THR:N	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:f:140:ILE:HG23	3:f:149:PHE:CD1	2.52	0.44
2:Q:31:ASP:OD1	2:Q:31:ASP:C	2.60	0.44
2:B:401:ARG:HB3	1:G:262:TYR:OH	2.17	0.44
2:D:31:ASP:C	2:D:31:ASP:OD1	2.60	0.44
1:P:358:GLN:O	1:P:359:PRO:C	2.60	0.44
1:R:358:GLN:O	1:R:359:PRO:C	2.60	0.44
3:b:18:ARG:HD2	3:b:18:ARG:O	2.17	0.44
1:G:358:GLN:O	1:G:359:PRO:C	2.60	0.44
1:I:358:GLN:O	1:I:359:PRO:C	2.60	0.44
3:e:18:ARG:HD2	3:e:18:ARG:O	2.17	0.44
3:f:18:ARG:HD2	3:f:18:ARG:O	2.17	0.44
2:B:220:THR:OG1	2:B:221:THR:N	2.50	0.44
3:b:140:ILE:HG23	3:b:149:PHE:CD1	2.52	0.44
1:L:367:ASP:O	1:L:368:LEU:C	2.59	0.44
2:S:31:ASP:OD1	2:S:31:ASP:C	2.61	0.44
1:C:172:TYR:HA	1:C:173:PRO:HD3	1.89	0.44
2:F:347:ILE:O	2:F:348:PRO:C	2.61	0.44
2:J:31:ASP:OD1	2:J:31:ASP:C	2.60	0.44
2:O:347:ILE:O	2:O:348:PRO:C	2.61	0.44
7:f:501:ANP:O2A	7:f:501:ANP:H8	2.18	0.44
1:P:172:TYR:HA	1:P:173:PRO:HD3	1.89	0.44
1:R:172:TYR:HA	1:R:173:PRO:HD3	1.89	0.44
1:A:358:GLN:O	1:A:359:PRO:C	2.60	0.44
2:B:31:ASP:OD1	2:B:31:ASP:C	2.60	0.44
1:E:367:ASP:O	1:E:368:LEU:C	2.59	0.44
7:b:501:ANP:O2A	7:b:501:ANP:H8	2.18	0.44
2:H:220:THR:OG1	2:H:221:THR:N	2.50	0.44
3:e:140:ILE:HG23	3:e:149:PHE:CD1	2.52	0.44
1:N:367:ASP:O	1:N:368:LEU:C	2.59	0.44
2:M:347:ILE:O	2:M:348:PRO:C	2.61	0.43
7:e:501:ANP:O2A	7:e:501:ANP:H8	2.18	0.43
2:H:31:ASP:OD1	2:H:31:ASP:C	2.61	0.43
1:I:290:GLU:OE2	1:R:124:LYS:HE3	2.18	0.43
1:L:358:GLN:O	1:L:359:PRO:C	2.60	0.43
1:N:358:GLN:O	1:N:359:PRO:C	2.60	0.43
2:D:11:GLN:HB2	6:D:501:G2P:O2A	2.18	0.43
2:D:220:THR:OG1	2:D:221:THR:N	2.50	0.43
1:E:358:GLN:O	1:E:359:PRO:C	2.60	0.43
2:F:11:GLN:HB2	6:F:501:G2P:O2A	2.18	0.43
2:J:220:THR:OG1	2:J:221:THR:N	2.50	0.43
2:M:11:GLN:HB2	6:M:501:G2P:O2A	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:220:THR:OG1	2:Q:221:THR:N	2.50	0.43
7:g:501:ANP:O2A	7:g:501:ANP:H8	2.18	0.43
2:S:220:THR:OG1	2:S:221:THR:N	2.50	0.43
7:h:501:ANP:O2A	7:h:501:ANP:H8	2.18	0.43
7:a:501:ANP:O2A	7:a:501:ANP:H8	2.18	0.43
2:H:11:GLN:HB2	6:H:501:G2P:O2A	2.18	0.43
2:M:31:ASP:C	2:M:31:ASP:OD1	2.60	0.43
2:Q:11:GLN:HB2	6:Q:501:G2P:O2A	2.18	0.43
2:B:11:GLN:HB2	6:B:501:G2P:O2A	2.18	0.43
2:F:31:ASP:C	2:F:31:ASP:OD1	2.60	0.43
7:d:501:ANP:O2A	7:d:501:ANP:H8	2.18	0.43
2:O:11:GLN:HB2	6:O:501:G2P:O2A	2.18	0.43
2:S:11:GLN:HB2	6:S:501:G2P:O2A	2.18	0.43
7:K:501:ANP:O2A	7:K:501:ANP:H8	2.18	0.43
7:c:501:ANP:O2A	7:c:501:ANP:H8	2.18	0.43
2:J:11:GLN:HB2	6:J:501:G2P:O2A	2.18	0.43
2:O:31:ASP:OD1	2:O:31:ASP:C	2.60	0.43
2:J:283:TYR:CD1	2:S:89:PRO:HD2	2.54	0.43
3:e:25:LYS:HA	3:e:28:LEU:HG	2.01	0.43
3:g:158:ILE:HB	3:g:228:HIS:HB2	2.01	0.43
3:a:158:ILE:HB	3:a:228:HIS:HB2	2.01	0.43
3:b:25:LYS:HA	3:b:28:LEU:HG	2.01	0.43
2:M:177:VAL:O	2:M:177:VAL:HG12	2.19	0.43
3:f:25:LYS:HA	3:f:28:LEU:HG	2.01	0.43
3:h:158:ILE:HB	3:h:228:HIS:HB2	2.01	0.43
2:F:177:VAL:O	2:F:177:VAL:HG12	2.19	0.43
1:G:2:ARG:O	1:G:2:ARG:HG3	2.19	0.43
1:I:2:ARG:O	1:I:2:ARG:HG3	2.19	0.43
1:A:2:ARG:HG3	1:A:2:ARG:O	2.19	0.42
2:D:83:PHE:HA	2:D:86:ILE:HB	2.01	0.42
2:O:177:VAL:O	2:O:177:VAL:HG12	2.19	0.42
2:B:83:PHE:HA	2:B:86:ILE:HB	2.01	0.42
2:H:83:PHE:HA	2:H:86:ILE:HB	2.02	0.42
2:J:83:PHE:HA	2:J:86:ILE:HB	2.01	0.42
2:Q:83:PHE:HA	2:Q:86:ILE:HB	2.01	0.42
2:S:83:PHE:HA	2:S:86:ILE:HB	2.02	0.42
2:F:40:SER:OG	2:F:41:ASP:N	2.53	0.42
1:G:172:TYR:HA	1:G:173:PRO:HD3	1.89	0.42
3:e:158:ILE:HB	3:e:228:HIS:HB2	2.01	0.42
1:N:49:PHE:CD1	1:N:49:PHE:C	2.97	0.42
1:A:1:MET:O	1:A:2:ARG:C	2.62	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:40:SER:OG	2:D:41:ASP:N	2.53	0.42
2:D:177:VAL:O	2:D:177:VAL:HG12	2.18	0.42
3:b:158:ILE:HB	3:b:228:HIS:HB2	2.01	0.42
1:I:1:MET:O	1:I:2:ARG:C	2.62	0.42
2:M:40:SER:OG	2:M:41:ASP:N	2.53	0.42
2:O:40:SER:OG	2:O:41:ASP:N	2.53	0.42
2:Q:40:SER:OG	2:Q:41:ASP:N	2.53	0.42
1:E:2:ARG:O	1:E:2:ARG:HG3	2.19	0.42
3:c:158:ILE:HB	3:c:228:HIS:HB2	2.01	0.42
3:f:158:ILE:HB	3:f:228:HIS:HB2	2.01	0.42
2:S:40:SER:OG	2:S:41:ASP:N	2.53	0.42
2:S:177:VAL:O	2:S:177:VAL:HG12	2.18	0.42
3:h:115:LYS:HB2	3:h:115:LYS:HZ1	1.85	0.42
3:a:115:LYS:HB2	3:a:115:LYS:HZ1	1.85	0.42
2:F:83:PHE:HA	2:F:86:ILE:HB	2.01	0.42
1:G:1:MET:O	1:G:2:ARG:C	2.62	0.42
3:d:158:ILE:HB	3:d:228:HIS:HB2	2.01	0.42
2:Q:177:VAL:O	2:Q:177:VAL:HG12	2.19	0.42
3:g:25:LYS:HA	3:g:28:LEU:HG	2.01	0.42
2:B:177:VAL:O	2:B:177:VAL:HG12	2.18	0.42
3:K:241:ILE:HB	3:K:311:HIS:HB2	2.01	0.42
1:E:49:PHE:CD1	1:E:49:PHE:C	2.97	0.42
1:I:49:PHE:CD1	1:I:49:PHE:C	2.97	0.42
1:L:2:ARG:O	1:L:2:ARG:HG3	2.19	0.42
1:L:49:PHE:CD1	1:L:49:PHE:C	2.97	0.42
2:M:83:PHE:HA	2:M:86:ILE:HB	2.02	0.42
1:R:49:PHE:CD1	1:R:49:PHE:C	2.97	0.42
1:R:324:VAL:HA	1:R:325:PRO:HD3	1.90	0.42
1:A:49:PHE:CD1	1:A:49:PHE:C	2.97	0.42
1:C:49:PHE:CD1	1:C:49:PHE:C	2.97	0.42
3:a:25:LYS:HA	3:a:28:LEU:HG	2.01	0.42
2:H:40:SER:OG	2:H:41:ASP:N	2.53	0.42
3:d:114:GLY:CA	7:d:501:ANP:O2A	2.68	0.42
1:N:1:MET:O	1:N:2:ARG:C	2.62	0.42
1:N:2:ARG:O	1:N:2:ARG:HG3	2.19	0.42
2:O:306:ASP:HA	2:O:307:PRO:HD3	1.88	0.42
2:B:40:SER:OG	2:B:41:ASP:N	2.53	0.42
3:K:25:LYS:HA	3:K:28:LEU:HG	2.01	0.42
1:G:49:PHE:CD1	1:G:49:PHE:C	2.97	0.42
2:J:177:VAL:O	2:J:177:VAL:HG12	2.19	0.42
2:J:188:THR:HA	2:J:425:MET:SD	2.60	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:e:171:THR:HA	3:e:172:PRO:HD3	1.91	0.42
2:O:83:PHE:HA	2:O:86:ILE:HB	2.02	0.42
1:P:49:PHE:CD1	1:P:49:PHE:C	2.97	0.42
1:R:2:ARG:HG3	1:R:2:ARG:O	2.19	0.42
2:B:188:THR:HA	2:B:425:MET:SD	2.60	0.42
3:K:197:GLY:CA	7:K:501:ANP:O2A	2.68	0.42
1:C:2:ARG:HG3	1:C:2:ARG:O	2.19	0.42
1:C:324:VAL:HA	1:C:325:PRO:HD3	1.90	0.42
3:c:114:GLY:CA	7:c:501:ANP:O2A	2.68	0.42
1:I:324:VAL:HA	1:I:325:PRO:HD3	1.90	0.42
2:J:40:SER:OG	2:J:41:ASP:N	2.53	0.42
3:d:25:LYS:HA	3:d:28:LEU:HG	2.01	0.42
1:N:324:VAL:HA	1:N:325:PRO:HD3	1.90	0.42
2:O:44:LEU:HA	2:O:49:ILE:HB	2.02	0.42
3:h:25:LYS:HA	3:h:28:LEU:HG	2.01	0.42
1:C:1:MET:O	1:C:2:ARG:C	2.62	0.41
2:D:44:LEU:HA	2:D:49:ILE:HB	2.02	0.41
1:E:1:MET:O	1:E:2:ARG:C	2.62	0.41
2:F:44:LEU:HA	2:F:49:ILE:HB	2.02	0.41
2:H:177:VAL:O	2:H:177:VAL:HG12	2.18	0.41
2:H:188:THR:HA	2:H:425:MET:SD	2.60	0.41
1:L:1:MET:O	1:L:2:ARG:C	2.62	0.41
2:M:44:LEU:HA	2:M:49:ILE:HB	2.02	0.41
1:P:1:MET:O	1:P:2:ARG:C	2.62	0.41
1:P:2:ARG:O	1:P:2:ARG:HG3	2.19	0.41
1:R:1:MET:O	1:R:2:ARG:C	2.62	0.41
1:A:324:VAL:HA	1:A:325:PRO:HD3	1.90	0.41
1:N:267:PHE:O	1:N:268:PRO:C	2.63	0.41
2:Q:44:LEU:HA	2:Q:49:ILE:HB	2.02	0.41
2:Q:359:PRO:HA	2:Q:360:PRO:HD3	1.84	0.41
2:S:44:LEU:HA	2:S:49:ILE:HB	2.02	0.41
3:c:25:LYS:HA	3:c:28:LEU:HG	2.01	0.41
1:L:267:PHE:O	1:L:268:PRO:C	2.63	0.41
2:M:188:THR:HA	2:M:425:MET:SD	2.60	0.41
1:P:267:PHE:O	1:P:268:PRO:C	2.63	0.41
2:Q:62:VAL:HA	2:Q:63:PRO:HD3	1.93	0.41
3:K:178:ASP:OD1	3:K:222:LYS:NZ	2.53	0.41
1:C:267:PHE:O	1:C:268:PRO:C	2.63	0.41
1:E:267:PHE:O	1:E:268:PRO:C	2.63	0.41
3:b:171:THR:HA	3:b:172:PRO:HD3	1.91	0.41
1:P:324:VAL:HA	1:P:325:PRO:HD3	1.90	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:267:PHE:O	1:R:268:PRO:C	2.63	0.41
1:A:267:PHE:O	1:A:268:PRO:C	2.63	0.41
2:F:188:THR:HA	2:F:425:MET:SD	2.60	0.41
1:G:267:PHE:O	1:G:268:PRO:C	2.63	0.41
2:S:359:PRO:HA	2:S:360:PRO:HD3	1.84	0.41
2:D:359:PRO:HA	2:D:360:PRO:HD3	1.84	0.41
1:E:324:VAL:HA	1:E:325:PRO:HD3	1.90	0.41
2:F:306:ASP:HA	2:F:307:PRO:HD3	1.88	0.41
2:O:359:PRO:HA	2:O:360:PRO:HD3	1.84	0.41
1:G:283:HIS:CB	1:P:88:HIS:HB3	2.50	0.41
1:I:267:PHE:O	1:I:268:PRO:C	2.63	0.41
2:O:188:THR:HA	2:O:425:MET:SD	2.60	0.41
3:f:171:THR:HA	3:f:172:PRO:HD3	1.91	0.41
2:B:199:ASP:OD1	2:B:200:GLU:N	2.54	0.41
2:D:62:VAL:HA	2:D:63:PRO:HD3	1.93	0.41
2:F:359:PRO:HA	2:F:360:PRO:HD3	1.84	0.41
1:G:324:VAL:HA	1:G:325:PRO:HD3	1.90	0.41
2:M:306:ASP:HA	2:M:307:PRO:HD3	1.88	0.41
1:A:324:VAL:HG11	2:J:221:THR:HB	2.02	0.41
1:C:375:VAL:O	1:C:375:VAL:HG13	2.21	0.41
2:D:188:THR:HA	2:D:425:MET:SD	2.60	0.41
2:F:199:ASP:OD1	2:F:200:GLU:N	2.54	0.41
2:H:199:ASP:OD1	2:H:200:GLU:N	2.54	0.41
3:c:24:GLU:O	3:c:28:LEU:HG	2.21	0.41
2:J:199:ASP:OD1	2:J:200:GLU:N	2.54	0.41
2:M:199:ASP:OD1	2:M:200:GLU:N	2.53	0.41
1:N:172:TYR:HA	1:N:173:PRO:HD3	1.89	0.41
2:O:199:ASP:OD1	2:O:200:GLU:N	2.53	0.41
1:P:375:VAL:O	1:P:375:VAL:HG13	2.21	0.41
2:Q:188:THR:HA	2:Q:425:MET:SD	2.60	0.41
1:R:375:VAL:O	1:R:375:VAL:HG13	2.21	0.41
2:S:62:VAL:HA	2:S:63:PRO:HD3	1.93	0.41
2:S:188:THR:HA	2:S:425:MET:SD	2.60	0.41
1:A:375:VAL:O	1:A:375:VAL:HG13	2.21	0.41
3:a:24:GLU:O	3:a:28:LEU:HG	2.21	0.41
3:b:111:THR:HG23	3:b:111:THR:O	2.21	0.41
1:G:375:VAL:O	1:G:375:VAL:HG13	2.21	0.41
1:I:375:VAL:O	1:I:375:VAL:HG13	2.21	0.41
2:M:359:PRO:HA	2:M:360:PRO:HD3	1.84	0.41
3:e:111:THR:HG23	3:e:111:THR:O	2.21	0.41
3:f:111:THR:O	3:f:111:THR:HG23	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:194:THR:HG23	3:K:194:THR:O	2.21	0.40
3:K:254:THR:HA	3:K:255:PRO:HD3	1.91	0.40
2:D:67:LEU:HD12	2:D:67:LEU:N	2.36	0.40
2:H:44:LEU:HA	2:H:49:ILE:HB	2.02	0.40
1:L:375:VAL:O	1:L:375:VAL:HG13	2.21	0.40
3:g:24:GLU:O	3:g:28:LEU:HG	2.21	0.40
2:S:67:LEU:HD12	2:S:67:LEU:N	2.36	0.40
3:h:24:GLU:O	3:h:28:LEU:HG	2.21	0.40
2:B:395:PHE:CD2	2:B:395:PHE:C	2.99	0.40
3:K:24:GLU:O	3:K:28:LEU:HG	2.21	0.40
1:E:375:VAL:O	1:E:375:VAL:HG13	2.21	0.40
2:J:44:LEU:HA	2:J:49:ILE:HB	2.02	0.40
3:d:24:GLU:O	3:d:28:LEU:HG	2.21	0.40
1:L:324:VAL:HA	1:L:325:PRO:HD3	1.90	0.40
2:Q:67:LEU:HD12	2:Q:67:LEU:N	2.36	0.40
2:H:67:LEU:HD12	2:H:67:LEU:N	2.36	0.40
3:c:111:THR:HG23	3:c:111:THR:O	2.21	0.40
2:J:67:LEU:HD12	2:J:67:LEU:N	2.36	0.40
2:J:395:PHE:CD2	2:J:395:PHE:C	2.99	0.40
3:d:111:THR:HG23	3:d:111:THR:O	2.21	0.40
3:e:24:GLU:O	3:e:28:LEU:HG	2.21	0.40
1:N:375:VAL:O	1:N:375:VAL:HG13	2.21	0.40
2:B:44:LEU:HA	2:B:49:ILE:HB	2.03	0.40
3:a:111:THR:HG23	3:a:111:THR:O	2.21	0.40
3:b:24:GLU:O	3:b:28:LEU:HG	2.21	0.40
2:H:395:PHE:CD2	2:H:395:PHE:C	2.99	0.40
2:O:94:PHE:CD2	2:O:94:PHE:N	2.90	0.40
3:f:114:GLY:CA	7:f:501:ANP:O2A	2.68	0.40
3:g:111:THR:HG23	3:g:111:THR:O	2.21	0.40
1:E:172:TYR:HA	1:E:173:PRO:HD3	1.89	0.40
2:F:94:PHE:CD2	2:F:94:PHE:N	2.90	0.40
1:L:172:TYR:HA	1:L:173:PRO:HD3	1.89	0.40
2:M:94:PHE:CD2	2:M:94:PHE:N	2.90	0.40
3:h:111:THR:HG23	3:h:111:THR:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	424/451 (94%)	389 (92%)	27 (6%)	8 (2%)	6	34
1	C	424/451 (94%)	389 (92%)	27 (6%)	8 (2%)	6	34
1	E	424/451 (94%)	389 (92%)	27 (6%)	8 (2%)	6	34
1	G	424/451 (94%)	389 (92%)	27 (6%)	8 (2%)	6	34
1	I	424/451 (94%)	389 (92%)	27 (6%)	8 (2%)	6	34
1	L	424/451 (94%)	389 (92%)	27 (6%)	8 (2%)	6	34
1	N	424/451 (94%)	389 (92%)	27 (6%)	8 (2%)	6	34
1	P	424/451 (94%)	389 (92%)	27 (6%)	8 (2%)	6	34
1	R	424/451 (94%)	389 (92%)	27 (6%)	8 (2%)	6	34
2	B	424/445 (95%)	396 (93%)	24 (6%)	4 (1%)	14	49
2	D	424/445 (95%)	396 (93%)	24 (6%)	4 (1%)	14	49
2	F	424/445 (95%)	396 (93%)	24 (6%)	4 (1%)	14	49
2	H	424/445 (95%)	396 (93%)	24 (6%)	4 (1%)	14	49
2	J	424/445 (95%)	396 (93%)	24 (6%)	4 (1%)	14	49
2	M	424/445 (95%)	396 (93%)	24 (6%)	4 (1%)	14	49
2	O	424/445 (95%)	396 (93%)	24 (6%)	4 (1%)	14	49
2	Q	424/445 (95%)	396 (93%)	23 (5%)	5 (1%)	10	42
2	S	424/445 (95%)	396 (93%)	23 (5%)	5 (1%)	10	42
3	K	326/355 (92%)	299 (92%)	24 (7%)	3 (1%)	14	49
3	a	326/355 (92%)	299 (92%)	24 (7%)	3 (1%)	14	49
3	b	326/355 (92%)	299 (92%)	24 (7%)	3 (1%)	14	49
3	c	326/355 (92%)	299 (92%)	24 (7%)	3 (1%)	14	49
3	d	326/355 (92%)	299 (92%)	24 (7%)	3 (1%)	14	49
3	e	326/355 (92%)	299 (92%)	24 (7%)	3 (1%)	14	49
3	f	326/355 (92%)	299 (92%)	24 (7%)	3 (1%)	14	49

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	g	326/355 (92%)	299 (92%)	24 (7%)	3 (1%)	14	49
3	h	326/355 (92%)	299 (92%)	24 (7%)	3 (1%)	14	49
All	All	10566/11259 (94%)	9756 (92%)	673 (6%)	137 (1%)	12	41

All (137) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	249	ASN
3	K	194	THR
3	K	203	SER
3	K	393	SER
2	D	249	ASN
3	a	111	THR
3	a	120	SER
3	a	310	SER
2	F	249	ASN
3	b	111	THR
3	b	120	SER
3	b	310	SER
2	H	249	ASN
3	c	111	THR
3	c	120	SER
3	c	310	SER
2	J	249	ASN
3	d	111	THR
3	d	120	SER
3	d	310	SER
2	M	249	ASN
3	e	111	THR
3	e	120	SER
3	e	310	SER
2	O	249	ASN
3	f	111	THR
3	f	120	SER
3	f	310	SER
2	Q	249	ASN
3	g	111	THR
3	g	120	SER
3	g	310	SER
2	S	249	ASN
3	h	111	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	h	120	SER
3	h	310	SER
2	B	348	PRO
2	D	348	PRO
2	F	348	PRO
2	H	348	PRO
2	J	348	PRO
2	M	348	PRO
2	O	348	PRO
2	Q	348	PRO
2	S	348	PRO
1	A	2	ARG
1	A	279	GLU
1	C	2	ARG
1	C	279	GLU
1	E	2	ARG
1	E	279	GLU
1	G	2	ARG
1	G	279	GLU
1	I	2	ARG
1	I	279	GLU
1	I	368	LEU
1	L	2	ARG
1	L	279	GLU
1	N	2	ARG
1	N	279	GLU
1	P	2	ARG
1	P	279	GLU
1	P	368	LEU
1	R	2	ARG
1	R	279	GLU
1	A	268	PRO
1	A	368	LEU
2	B	222	PRO
1	C	268	PRO
1	C	368	LEU
2	D	222	PRO
1	E	268	PRO
1	E	368	LEU
2	F	222	PRO
1	G	268	PRO
1	G	368	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	222	PRO
1	I	268	PRO
2	J	222	PRO
1	L	268	PRO
1	L	368	LEU
2	M	222	PRO
1	N	268	PRO
1	N	368	LEU
2	O	222	PRO
1	P	268	PRO
2	Q	222	PRO
1	R	268	PRO
1	R	368	LEU
2	S	222	PRO
1	A	359	PRO
1	C	359	PRO
1	E	359	PRO
1	G	359	PRO
1	I	359	PRO
1	L	359	PRO
1	N	359	PRO
1	P	359	PRO
1	R	359	PRO
1	A	267	PHE
1	A	364	PRO
1	C	267	PHE
1	C	364	PRO
1	E	267	PHE
1	E	364	PRO
1	G	267	PHE
1	G	364	PRO
1	I	267	PHE
1	I	364	PRO
1	L	267	PHE
1	L	364	PRO
1	N	267	PHE
1	N	364	PRO
1	P	267	PHE
1	P	364	PRO
1	R	267	PHE
1	R	364	PRO
2	B	307	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	307	PRO
2	F	307	PRO
2	H	307	PRO
2	J	307	PRO
2	M	307	PRO
2	O	307	PRO
2	Q	307	PRO
2	S	307	PRO
2	Q	72	PRO
2	S	72	PRO
1	A	274	PRO
1	L	274	PRO
1	N	274	PRO
1	P	274	PRO
1	R	274	PRO
1	C	274	PRO
1	E	274	PRO
1	G	274	PRO
1	I	274	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	66/379 (17%)	65 (98%)	1 (2%)	57	70
1	G	126/379 (33%)	126 (100%)	0	100	100
1	L	362/379 (96%)	359 (99%)	3 (1%)	73	77
1	N	362/379 (96%)	359 (99%)	3 (1%)	73	77
1	P	362/379 (96%)	359 (99%)	3 (1%)	73	77
1	R	362/379 (96%)	359 (99%)	3 (1%)	73	77
2	F	8/381 (2%)	8 (100%)	0	100	100
2	H	69/381 (18%)	67 (97%)	2 (3%)	37	58
2	J	269/381 (71%)	265 (98%)	4 (2%)	57	70

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	M	367/381 (96%)	362 (99%)	5 (1%)	59	71
2	O	367/381 (96%)	362 (99%)	5 (1%)	59	71
2	Q	367/381 (96%)	362 (99%)	5 (1%)	59	71
2	S	367/381 (96%)	362 (99%)	5 (1%)	59	71
3	K	217/319 (68%)	217 (100%)	0	100	100
3	b	200/319 (63%)	198 (99%)	2 (1%)	68	76
3	d	295/319 (92%)	293 (99%)	2 (1%)	76	79
3	e	295/319 (92%)	293 (99%)	2 (1%)	76	79
3	f	295/319 (92%)	293 (99%)	2 (1%)	76	79
3	g	295/319 (92%)	293 (99%)	2 (1%)	76	79
3	h	295/319 (92%)	293 (99%)	2 (1%)	76	79
All	All	5346/7174 (74%)	5295 (99%)	51 (1%)	65	76

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	32	PRO
3	b	115	LYS
3	b	123	PRO
2	H	89	PRO
2	H	184	PRO
2	J	32	PRO
2	J	89	PRO
2	J	263	PRO
2	J	289	PRO
3	d	115	LYS
3	d	123	PRO
1	L	32	PRO
1	L	89	PRO
1	L	175	PRO
2	M	32	PRO
2	M	89	PRO
2	M	184	PRO
2	M	263	PRO
2	M	289	PRO
3	e	115	LYS
3	e	123	PRO
1	N	32	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	89	PRO
1	N	175	PRO
2	O	32	PRO
2	O	89	PRO
2	O	184	PRO
2	O	263	PRO
2	O	289	PRO
3	f	115	LYS
3	f	123	PRO
1	P	32	PRO
1	P	89	PRO
1	P	175	PRO
2	Q	32	PRO
2	Q	89	PRO
2	Q	184	PRO
2	Q	263	PRO
2	Q	289	PRO
3	g	115	LYS
3	g	123	PRO
1	R	32	PRO
1	R	89	PRO
1	R	175	PRO
2	S	32	PRO
2	S	89	PRO
2	S	184	PRO
2	S	263	PRO
2	S	289	PRO
3	h	115	LYS
3	h	123	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
3	K	304	ASN
3	K	362	ASN
1	C	11	GLN
1	C	31	GLN
3	b	221	ASN
3	b	279	ASN
1	G	11	GLN
1	G	133	GLN
2	J	385	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	d	221	ASN
3	d	279	ASN
1	L	11	GLN
1	L	31	GLN
1	L	133	GLN
1	L	226	ASN
1	L	285	GLN
1	L	393	HIS
1	L	406	HIS
2	M	8	GLN
2	M	15	GLN
2	M	136	GLN
2	M	385	GLN
3	e	221	ASN
3	e	279	ASN
1	N	11	GLN
1	N	31	GLN
1	N	133	GLN
1	N	226	ASN
1	N	393	HIS
1	N	406	HIS
2	O	8	GLN
2	O	15	GLN
2	O	136	GLN
2	O	385	GLN
3	f	221	ASN
3	f	279	ASN
1	P	11	GLN
1	P	31	GLN
1	P	133	GLN
1	P	226	ASN
1	P	393	HIS
1	P	406	HIS
2	Q	8	GLN
2	Q	15	GLN
2	Q	136	GLN
2	Q	385	GLN
3	g	221	ASN
3	g	279	ASN
1	R	11	GLN
1	R	31	GLN
1	R	133	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	R	226	ASN
1	R	393	HIS
1	R	406	HIS
2	S	8	GLN
2	S	15	GLN
2	S	136	GLN
2	S	385	GLN
3	h	221	ASN
3	h	279	ASN

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](#)

Of 54 ligands modelled in this entry, 27 are monoatomic - leaving 27 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	ANP	c	501	5	33,33,33	1.97	9 (27%)	45,52,52	3.16	24 (53%)
6	G2P	S	501	5	30,34,34	1.84	8 (26%)	46,54,54	2.20	14 (30%)
6	G2P	O	501	5	30,34,34	1.84	7 (23%)	46,54,54	2.21	14 (30%)
7	ANP	b	501	5	33,33,33	1.97	10 (30%)	45,52,52	3.16	24 (53%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	G2P	B	501	5	30,34,34	1.85	7 (23%)	46,54,54	2.20	14 (30%)
6	G2P	D	501	5	30,34,34	1.85	8 (26%)	46,54,54	2.21	14 (30%)
7	ANP	e	501	5	33,33,33	1.97	10 (30%)	45,52,52	3.15	25 (55%)
6	G2P	M	501	5	30,34,34	1.85	7 (23%)	46,54,54	2.20	14 (30%)
7	ANP	h	501	5	33,33,33	1.98	10 (30%)	45,52,52	3.15	23 (51%)
6	G2P	F	501	5	30,34,34	1.84	7 (23%)	46,54,54	2.20	14 (30%)
4	GTP	G	501	5	33,34,34	1.13	4 (12%)	50,54,54	1.68	7 (14%)
6	G2P	J	501	5	30,34,34	1.84	7 (23%)	46,54,54	2.20	14 (30%)
4	GTP	C	501	5	33,34,34	1.12	4 (12%)	50,54,54	1.68	7 (14%)
4	GTP	L	501	5	33,34,34	1.13	4 (12%)	50,54,54	1.67	7 (14%)
7	ANP	f	501	5	33,33,33	1.97	10 (30%)	45,52,52	3.16	24 (53%)
6	G2P	Q	501	5	30,34,34	1.83	7 (23%)	46,54,54	2.20	13 (28%)
4	GTP	N	501	5	33,34,34	1.13	4 (12%)	50,54,54	1.68	7 (14%)
6	G2P	H	501	5	30,34,34	1.85	8 (26%)	46,54,54	2.21	14 (30%)
7	ANP	d	501	5	33,33,33	1.98	10 (30%)	45,52,52	3.15	24 (53%)
4	GTP	I	501	5	33,34,34	1.14	4 (12%)	50,54,54	1.68	7 (14%)
7	ANP	a	501	5	33,33,33	1.97	9 (27%)	45,52,52	3.15	23 (51%)
7	ANP	K	501	5	33,33,33	1.98	10 (30%)	45,52,52	3.15	24 (53%)
4	GTP	R	501	5	33,34,34	1.14	4 (12%)	50,54,54	1.68	7 (14%)
4	GTP	A	501	5	33,34,34	1.13	4 (12%)	50,54,54	1.67	7 (14%)
4	GTP	P	501	5	33,34,34	1.13	4 (12%)	50,54,54	1.67	7 (14%)
4	GTP	E	501	5	33,34,34	1.12	4 (12%)	50,54,54	1.67	7 (14%)
7	ANP	g	501	5	33,33,33	1.97	10 (30%)	45,52,52	3.15	24 (53%)

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
7	ANP	c	501	5	-	3/18/38/38	0/3/3/3
6	G2P	S	501	5	-	4/19/38/38	0/3/3/3
6	G2P	O	501	5	-	4/19/38/38	0/3/3/3
7	ANP	b	501	5	-	3/18/38/38	0/3/3/3
6	G2P	B	501	5	-	4/19/38/38	0/3/3/3
6	G2P	D	501	5	-	4/19/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	ANP	e	501	5	-	3/18/38/38	0/3/3/3
6	G2P	M	501	5	-	4/19/38/38	0/3/3/3
7	ANP	h	501	5	-	3/18/38/38	0/3/3/3
6	G2P	F	501	5	-	4/19/38/38	0/3/3/3
4	GTP	G	501	5	-	7/22/38/38	0/3/3/3
6	G2P	J	501	5	-	4/19/38/38	0/3/3/3
4	GTP	C	501	5	-	7/22/38/38	0/3/3/3
4	GTP	L	501	5	-	7/22/38/38	0/3/3/3
7	ANP	f	501	5	-	3/18/38/38	0/3/3/3
6	G2P	Q	501	5	-	4/19/38/38	0/3/3/3
4	GTP	N	501	5	-	7/22/38/38	0/3/3/3
6	G2P	H	501	5	-	4/19/38/38	0/3/3/3
7	ANP	d	501	5	-	3/18/38/38	0/3/3/3
4	GTP	I	501	5	-	7/22/38/38	0/3/3/3
7	ANP	a	501	5	-	3/18/38/38	0/3/3/3
7	ANP	K	501	5	-	3/18/38/38	0/3/3/3
4	GTP	R	501	5	-	7/22/38/38	0/3/3/3
4	GTP	A	501	5	-	7/22/38/38	0/3/3/3
4	GTP	P	501	5	-	7/22/38/38	0/3/3/3
4	GTP	E	501	5	-	7/22/38/38	0/3/3/3
7	ANP	g	501	5	-	3/18/38/38	0/3/3/3

All (190) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	d	501	ANP	PA-O3A	-5.73	1.53	1.59
7	K	501	ANP	PA-O3A	-5.70	1.53	1.59
7	h	501	ANP	PA-O3A	-5.68	1.53	1.59
7	c	501	ANP	PA-O3A	-5.67	1.53	1.59
7	b	501	ANP	PA-O3A	-5.65	1.53	1.59
7	a	501	ANP	PA-O3A	-5.65	1.53	1.59
7	f	501	ANP	PA-O3A	-5.61	1.53	1.59
7	e	501	ANP	PA-O3A	-5.61	1.53	1.59
7	g	501	ANP	PA-O3A	-5.61	1.53	1.59
7	e	501	ANP	PG-O1G	4.79	1.53	1.46
7	K	501	ANP	PG-O1G	4.79	1.53	1.46
7	c	501	ANP	PG-O1G	4.78	1.53	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	f	501	ANP	PG-O1G	4.77	1.53	1.46
7	d	501	ANP	PG-O1G	4.76	1.53	1.46
7	b	501	ANP	PG-O1G	4.75	1.53	1.46
7	g	501	ANP	PG-O1G	4.74	1.53	1.46
7	h	501	ANP	PG-O1G	4.73	1.53	1.46
7	a	501	ANP	PG-O1G	4.70	1.53	1.46
6	B	501	G2P	PB-O2B	4.35	1.61	1.51
6	F	501	G2P	PB-O2B	4.33	1.61	1.51
6	H	501	G2P	PB-O2B	4.33	1.61	1.51
6	M	501	G2P	PB-O2B	4.31	1.61	1.51
6	J	501	G2P	PB-O2B	4.30	1.61	1.51
6	Q	501	G2P	PB-O2B	4.30	1.61	1.51
6	O	501	G2P	PB-O2B	4.28	1.61	1.51
6	S	501	G2P	PB-O2B	4.28	1.61	1.51
6	B	501	G2P	PA-O2A	4.28	1.61	1.51
6	J	501	G2P	PA-O2A	4.28	1.61	1.51
6	M	501	G2P	PA-O2A	4.28	1.61	1.51
6	D	501	G2P	PA-O2A	4.28	1.61	1.51
6	O	501	G2P	PA-O2A	4.27	1.61	1.51
6	D	501	G2P	PB-O2B	4.27	1.61	1.51
6	S	501	G2P	PA-O2A	4.27	1.61	1.51
6	Q	501	G2P	PA-O2A	4.26	1.61	1.51
6	F	501	G2P	PA-O2A	4.26	1.61	1.51
6	H	501	G2P	PA-O2A	4.25	1.61	1.51
7	b	501	ANP	PA-O5'	3.95	1.74	1.59
7	f	501	ANP	PA-O5'	3.95	1.74	1.59
7	d	501	ANP	PA-O5'	3.95	1.74	1.59
7	g	501	ANP	PA-O5'	3.94	1.74	1.59
7	e	501	ANP	PA-O5'	3.93	1.74	1.59
7	h	501	ANP	PA-O5'	3.93	1.74	1.59
7	a	501	ANP	PA-O5'	3.93	1.74	1.59
7	K	501	ANP	PA-O5'	3.92	1.74	1.59
7	c	501	ANP	PA-O5'	3.91	1.74	1.59
6	B	501	G2P	PB-O1B	-3.48	1.47	1.56
6	M	501	G2P	PB-O1B	-3.48	1.47	1.56
6	S	501	G2P	PB-O1B	-3.47	1.47	1.56
6	H	501	G2P	PB-O1B	-3.46	1.47	1.56
6	D	501	G2P	PB-O1B	-3.46	1.47	1.56
6	F	501	G2P	PB-O1B	-3.44	1.48	1.56
6	Q	501	G2P	PB-O1B	-3.44	1.48	1.56
6	J	501	G2P	PB-O1B	-3.44	1.48	1.56
6	O	501	G2P	PB-O1B	-3.42	1.48	1.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	501	G2P	PA-O1A	-3.23	1.48	1.56
6	H	501	G2P	PA-O1A	-3.21	1.48	1.56
6	B	501	G2P	PA-O1A	-3.20	1.48	1.56
6	S	501	G2P	PA-O1A	-3.20	1.48	1.56
6	M	501	G2P	PA-O1A	-3.20	1.48	1.56
6	O	501	G2P	PA-O1A	-3.20	1.48	1.56
6	J	501	G2P	PA-O1A	-3.19	1.48	1.56
6	F	501	G2P	PA-O1A	-3.18	1.48	1.56
7	e	501	ANP	O5'-C5'	-3.15	1.32	1.44
7	a	501	ANP	O5'-C5'	-3.15	1.32	1.44
6	Q	501	G2P	PA-O1A	-3.15	1.48	1.56
7	h	501	ANP	O5'-C5'	-3.14	1.32	1.44
7	b	501	ANP	O5'-C5'	-3.14	1.32	1.44
7	f	501	ANP	O5'-C5'	-3.14	1.32	1.44
7	c	501	ANP	O5'-C5'	-3.13	1.32	1.44
7	d	501	ANP	O5'-C5'	-3.13	1.32	1.44
7	g	501	ANP	O5'-C5'	-3.13	1.32	1.44
7	K	501	ANP	O5'-C5'	-3.12	1.32	1.44
6	B	501	G2P	C5-C4	2.97	1.46	1.38
6	H	501	G2P	C5-C4	2.96	1.46	1.38
6	F	501	G2P	C5-C4	2.95	1.46	1.38
6	D	501	G2P	C5-C4	2.95	1.46	1.38
6	M	501	G2P	C5-C4	2.94	1.46	1.38
6	Q	501	G2P	C5-C4	2.94	1.46	1.38
6	O	501	G2P	C5-C4	2.94	1.46	1.38
6	S	501	G2P	C5-C4	2.93	1.46	1.38
6	J	501	G2P	C5-C4	2.93	1.46	1.38
4	N	501	GTP	C5-C4	2.87	1.46	1.38
4	I	501	GTP	C5-C4	2.86	1.46	1.38
4	C	501	GTP	C5-C4	2.86	1.46	1.38
4	L	501	GTP	C5-C4	2.85	1.46	1.38
4	G	501	GTP	C5-C4	2.84	1.46	1.38
4	R	501	GTP	C5-C4	2.84	1.46	1.38
4	A	501	GTP	C5-C4	2.83	1.46	1.38
4	E	501	GTP	C5-C4	2.82	1.46	1.38
4	P	501	GTP	C5-C4	2.81	1.46	1.38
6	B	501	G2P	C6-N1	-2.74	1.33	1.38
6	H	501	G2P	C6-N1	-2.72	1.33	1.38
6	M	501	G2P	C6-N1	-2.71	1.33	1.38
6	F	501	G2P	C6-N1	-2.70	1.33	1.38
6	D	501	G2P	C6-N1	-2.69	1.33	1.38
6	J	501	G2P	C6-N1	-2.69	1.33	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	O	501	G2P	C6-N1	-2.68	1.33	1.38
6	S	501	G2P	C6-N1	-2.66	1.33	1.38
6	Q	501	G2P	C6-N1	-2.65	1.33	1.38
4	R	501	GTP	C5-N7	-2.60	1.33	1.39
4	I	501	GTP	C5-N7	-2.60	1.33	1.39
4	G	501	GTP	C5-N7	-2.57	1.33	1.39
4	P	501	GTP	C5-N7	-2.55	1.34	1.39
4	L	501	GTP	C5-N7	-2.54	1.34	1.39
4	P	501	GTP	C6-N1	-2.52	1.34	1.38
4	L	501	GTP	C6-N1	-2.52	1.34	1.38
4	N	501	GTP	C5-N7	-2.51	1.34	1.39
4	C	501	GTP	C5-N7	-2.51	1.34	1.39
4	E	501	GTP	C5-N7	-2.50	1.34	1.39
4	A	501	GTP	C5-N7	-2.50	1.34	1.39
4	A	501	GTP	C6-N1	-2.50	1.34	1.38
6	O	501	G2P	C5-N7	-2.50	1.34	1.39
4	R	501	GTP	C6-N1	-2.49	1.34	1.38
4	I	501	GTP	C6-N1	-2.49	1.34	1.38
6	D	501	G2P	C5-N7	-2.49	1.34	1.39
6	J	501	G2P	C5-N7	-2.49	1.34	1.39
4	E	501	GTP	C6-N1	-2.49	1.34	1.38
4	N	501	GTP	C6-N1	-2.48	1.34	1.38
4	G	501	GTP	C6-N1	-2.48	1.34	1.38
6	M	501	G2P	C5-N7	-2.48	1.34	1.39
6	Q	501	G2P	C5-N7	-2.47	1.34	1.39
4	C	501	GTP	C6-N1	-2.47	1.34	1.38
6	B	501	G2P	C5-N7	-2.46	1.34	1.39
6	S	501	G2P	C5-N7	-2.46	1.34	1.39
6	H	501	G2P	C5-N7	-2.46	1.34	1.39
6	F	501	G2P	C5-N7	-2.44	1.34	1.39
7	b	501	ANP	PB-N3B	2.44	1.69	1.63
7	h	501	ANP	PG-O3G	-2.43	1.50	1.56
7	c	501	ANP	PG-O3G	-2.43	1.50	1.56
7	a	501	ANP	PB-N3B	2.43	1.69	1.63
7	f	501	ANP	PB-N3B	2.42	1.69	1.63
7	K	501	ANP	PB-N3B	2.42	1.69	1.63
7	e	501	ANP	PG-O3G	-2.40	1.50	1.56
7	d	501	ANP	PB-N3B	2.40	1.69	1.63
7	d	501	ANP	PG-O3G	-2.40	1.50	1.56
7	g	501	ANP	PG-O3G	-2.40	1.50	1.56
7	c	501	ANP	PB-N3B	2.40	1.69	1.63
7	a	501	ANP	PG-O3G	-2.40	1.50	1.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	h	501	ANP	PB-N3B	2.39	1.69	1.63
4	R	501	GTP	C4-N9	-2.39	1.32	1.38
4	N	501	GTP	C4-N9	-2.39	1.32	1.38
7	K	501	ANP	PG-O3G	-2.39	1.50	1.56
4	I	501	GTP	C4-N9	-2.38	1.32	1.38
7	h	501	ANP	C5-N7	-2.38	1.34	1.39
7	b	501	ANP	PG-O3G	-2.38	1.50	1.56
4	C	501	GTP	C4-N9	-2.37	1.32	1.38
7	g	501	ANP	PB-N3B	2.37	1.69	1.63
4	A	501	GTP	C4-N9	-2.36	1.32	1.38
7	f	501	ANP	PG-O3G	-2.36	1.50	1.56
4	E	501	GTP	C4-N9	-2.36	1.32	1.38
7	e	501	ANP	PB-N3B	2.36	1.69	1.63
4	G	501	GTP	C4-N9	-2.36	1.32	1.38
4	L	501	GTP	C4-N9	-2.35	1.32	1.38
7	f	501	ANP	C5-N7	-2.35	1.34	1.39
4	P	501	GTP	C4-N9	-2.35	1.32	1.38
7	K	501	ANP	C5-N7	-2.33	1.34	1.39
7	b	501	ANP	C5-N7	-2.31	1.34	1.39
7	d	501	ANP	C5-N7	-2.30	1.34	1.39
7	a	501	ANP	C5-N7	-2.29	1.34	1.39
7	g	501	ANP	C5-N7	-2.29	1.34	1.39
7	c	501	ANP	C5-N7	-2.27	1.34	1.39
7	e	501	ANP	C5-N7	-2.27	1.34	1.39
7	a	501	ANP	C1'-N9	-2.21	1.40	1.46
7	b	501	ANP	C1'-N9	-2.20	1.40	1.46
7	g	501	ANP	C1'-N9	-2.20	1.40	1.46
7	e	501	ANP	C1'-N9	-2.19	1.40	1.46
7	c	501	ANP	C1'-N9	-2.18	1.40	1.46
7	h	501	ANP	C1'-N9	-2.18	1.40	1.46
7	d	501	ANP	C1'-N9	-2.18	1.40	1.46
7	K	501	ANP	C1'-N9	-2.16	1.40	1.46
7	f	501	ANP	C1'-N9	-2.15	1.40	1.46
7	g	501	ANP	PG-O2G	-2.08	1.51	1.56
7	e	501	ANP	PG-O2G	-2.05	1.51	1.56
7	f	501	ANP	PG-O2G	-2.05	1.51	1.56
7	h	501	ANP	PG-O2G	-2.04	1.51	1.56
7	a	501	ANP	PG-O2G	-2.04	1.51	1.56
6	D	501	G2P	PB-O3B	2.04	1.60	1.58
7	K	501	ANP	PG-O2G	-2.04	1.51	1.56
7	b	501	ANP	PG-O2G	-2.04	1.51	1.56
7	d	501	ANP	PG-O2G	-2.03	1.51	1.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	e	501	ANP	O4'-C1'	2.03	1.46	1.42
7	g	501	ANP	O4'-C1'	2.02	1.46	1.42
7	f	501	ANP	O4'-C1'	2.02	1.46	1.42
7	K	501	ANP	O4'-C1'	2.02	1.46	1.42
7	h	501	ANP	O4'-C1'	2.01	1.46	1.42
7	c	501	ANP	PG-O2G	-2.01	1.51	1.56
6	S	501	G2P	PB-O3B	2.00	1.60	1.58
7	d	501	ANP	O4'-C1'	2.00	1.46	1.42
7	b	501	ANP	O4'-C1'	2.00	1.46	1.42
6	H	501	G2P	C4-N9	-2.00	1.33	1.38

All (403) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	K	501	ANP	C5'-C4'-C3'	-7.56	87.99	115.21
7	g	501	ANP	C5'-C4'-C3'	-7.56	88.01	115.21
7	a	501	ANP	C5'-C4'-C3'	-7.55	88.02	115.21
7	d	501	ANP	C5'-C4'-C3'	-7.55	88.03	115.21
7	h	501	ANP	C5'-C4'-C3'	-7.55	88.04	115.21
7	e	501	ANP	C5'-C4'-C3'	-7.55	88.05	115.21
7	b	501	ANP	C5'-C4'-C3'	-7.54	88.06	115.21
7	c	501	ANP	C5'-C4'-C3'	-7.54	88.07	115.21
7	f	501	ANP	C5'-C4'-C3'	-7.54	88.08	115.21
6	H	501	G2P	C5-C4-N3	-6.22	118.49	128.39
6	F	501	G2P	C5-C4-N3	-6.21	118.51	128.39
6	D	501	G2P	C5-C4-N3	-6.20	118.52	128.39
6	B	501	G2P	C5-C4-N3	-6.18	118.55	128.39
6	O	501	G2P	C5-C4-N3	-6.18	118.55	128.39
6	Q	501	G2P	C5-C4-N3	-6.18	118.55	128.39
6	J	501	G2P	C5-C4-N3	-6.17	118.56	128.39
6	S	501	G2P	C5-C4-N3	-6.17	118.57	128.39
6	M	501	G2P	C5-C4-N3	-6.15	118.60	128.39
7	h	501	ANP	O5'-C5'-C4'	6.02	129.50	108.99
7	e	501	ANP	O5'-C5'-C4'	6.02	129.49	108.99
7	c	501	ANP	O5'-C5'-C4'	6.02	129.48	108.99
7	a	501	ANP	O5'-C5'-C4'	6.01	129.47	108.99
7	b	501	ANP	O5'-C5'-C4'	6.01	129.46	108.99
7	f	501	ANP	O5'-C5'-C4'	6.01	129.45	108.99
7	d	501	ANP	O5'-C5'-C4'	6.01	129.44	108.99
7	g	501	ANP	O5'-C5'-C4'	6.00	129.43	108.99
7	K	501	ANP	O5'-C5'-C4'	6.00	129.41	108.99
7	f	501	ANP	O4'-C1'-N9	5.91	119.45	108.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	b	501	ANP	O4'-C1'-N9	5.90	119.42	108.09
7	c	501	ANP	O4'-C1'-N9	5.90	119.42	108.09
7	d	501	ANP	O4'-C1'-N9	5.89	119.41	108.09
7	a	501	ANP	O4'-C1'-N9	5.89	119.41	108.09
7	e	501	ANP	O4'-C1'-N9	5.88	119.38	108.09
7	g	501	ANP	O4'-C1'-N9	5.88	119.38	108.09
7	h	501	ANP	O4'-C1'-N9	5.88	119.38	108.09
7	K	501	ANP	O4'-C1'-N9	5.85	119.33	108.09
4	C	501	GTP	C5-C4-N3	-5.65	119.39	128.39
4	G	501	GTP	C5-C4-N3	-5.64	119.42	128.39
4	P	501	GTP	C5-C4-N3	-5.64	119.42	128.39
4	E	501	GTP	C5-C4-N3	-5.62	119.44	128.39
4	N	501	GTP	C5-C4-N3	-5.62	119.44	128.39
4	I	501	GTP	C5-C4-N3	-5.62	119.44	128.39
4	R	501	GTP	C5-C4-N3	-5.62	119.44	128.39
4	A	501	GTP	C5-C4-N3	-5.62	119.45	128.39
4	L	501	GTP	C5-C4-N3	-5.59	119.49	128.39
7	f	501	ANP	C5-C4-N3	-5.32	119.39	126.72
7	d	501	ANP	C5-C4-N3	-5.31	119.40	126.72
7	c	501	ANP	C5-C4-N3	-5.31	119.41	126.72
7	b	501	ANP	C5-C4-N3	-5.31	119.41	126.72
7	K	501	ANP	C5-C4-N3	-5.29	119.43	126.72
7	g	501	ANP	C5-C4-N3	-5.28	119.44	126.72
7	e	501	ANP	C5-C4-N3	-5.28	119.45	126.72
7	h	501	ANP	C5-C4-N3	-5.26	119.47	126.72
7	a	501	ANP	C5-C4-N3	-5.26	119.48	126.72
7	b	501	ANP	O3A-PB-N3B	-5.24	92.06	106.59
7	c	501	ANP	O3A-PB-N3B	-5.23	92.08	106.59
7	e	501	ANP	O3A-PB-N3B	-5.23	92.08	106.59
7	f	501	ANP	O3A-PB-N3B	-5.23	92.09	106.59
7	h	501	ANP	O3A-PB-N3B	-5.22	92.10	106.59
7	g	501	ANP	O3A-PB-N3B	-5.22	92.10	106.59
7	K	501	ANP	O3A-PB-N3B	-5.22	92.11	106.59
7	a	501	ANP	O3A-PB-N3B	-5.21	92.13	106.59
7	d	501	ANP	O3A-PB-N3B	-5.21	92.13	106.59
6	H	501	G2P	C2-N3-C4	5.12	121.12	112.30
6	O	501	G2P	C2-N3-C4	5.10	121.09	112.30
6	D	501	G2P	C2-N3-C4	5.09	121.06	112.30
7	h	501	ANP	O2A-PA-O3A	5.08	121.01	107.27
6	Q	501	G2P	C2-N3-C4	5.08	121.05	112.30
7	g	501	ANP	O2A-PA-O3A	5.08	121.00	107.27
7	e	501	ANP	N3-C2-N1	-5.08	120.90	128.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	K	501	ANP	O2A-PA-O3A	5.07	120.98	107.27
7	c	501	ANP	O2A-PA-O3A	5.07	120.98	107.27
7	b	501	ANP	O2A-PA-O3A	5.07	120.98	107.27
6	S	501	G2P	C2-N3-C4	5.07	121.03	112.30
6	F	501	G2P	C2-N3-C4	5.06	121.02	112.30
7	f	501	ANP	O2A-PA-O3A	5.06	120.94	107.27
7	d	501	ANP	O2A-PA-O3A	5.05	120.93	107.27
7	e	501	ANP	O2A-PA-O3A	5.05	120.91	107.27
7	b	501	ANP	N3-C2-N1	-5.05	120.94	128.58
7	c	501	ANP	N3-C2-N1	-5.05	120.94	128.58
6	J	501	G2P	C2-N3-C4	5.04	120.99	112.30
6	B	501	G2P	C2-N3-C4	5.04	120.99	112.30
6	M	501	G2P	C2-N3-C4	5.04	120.98	112.30
7	d	501	ANP	N3-C2-N1	-5.04	120.95	128.58
7	a	501	ANP	O2A-PA-O3A	5.04	120.89	107.27
7	h	501	ANP	N3-C2-N1	-5.03	120.96	128.58
7	f	501	ANP	N3-C2-N1	-5.03	120.97	128.58
7	K	501	ANP	N3-C2-N1	-5.01	121.00	128.58
7	a	501	ANP	N3-C2-N1	-5.01	121.00	128.58
7	g	501	ANP	N3-C2-N1	-5.00	121.01	128.58
7	f	501	ANP	N3-C4-N9	4.87	135.46	127.17
7	d	501	ANP	O2A-PA-O5'	-4.85	85.56	107.57
7	e	501	ANP	O2A-PA-O5'	-4.85	85.58	107.57
7	f	501	ANP	O2A-PA-O5'	-4.85	85.59	107.57
7	b	501	ANP	N3-C4-N9	4.85	135.41	127.17
7	a	501	ANP	O2A-PA-O5'	-4.84	85.61	107.57
7	c	501	ANP	O2A-PA-O5'	-4.84	85.62	107.57
7	b	501	ANP	O2A-PA-O5'	-4.84	85.63	107.57
7	h	501	ANP	O2A-PA-O5'	-4.84	85.64	107.57
7	g	501	ANP	O2A-PA-O5'	-4.83	85.66	107.57
7	K	501	ANP	O2A-PA-O5'	-4.83	85.66	107.57
4	G	501	GTP	C2-N3-C4	4.83	120.61	112.30
7	c	501	ANP	N3-C4-N9	4.82	135.37	127.17
7	a	501	ANP	N3-C4-N9	4.82	135.36	127.17
4	I	501	GTP	C2-N3-C4	4.82	120.60	112.30
7	d	501	ANP	N3-C4-N9	4.82	135.36	127.17
7	g	501	ANP	N3-C4-N9	4.82	135.36	127.17
4	C	501	GTP	C2-N3-C4	4.81	120.58	112.30
7	K	501	ANP	N3-C4-N9	4.81	135.35	127.17
7	h	501	ANP	N3-C4-N9	4.81	135.34	127.17
4	A	501	GTP	C2-N3-C4	4.80	120.56	112.30
4	E	501	GTP	C2-N3-C4	4.79	120.54	112.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	N	501	GTP	C2-N3-C4	4.79	120.54	112.30
7	e	501	ANP	N3-C4-N9	4.78	135.30	127.17
4	P	501	GTP	C2-N3-C4	4.78	120.53	112.30
4	R	501	GTP	C2-N3-C4	4.78	120.53	112.30
4	L	501	GTP	C2-N3-C4	4.76	120.49	112.30
7	b	501	ANP	O5'-PA-O1A	-4.68	90.39	108.94
7	g	501	ANP	O5'-PA-O1A	-4.68	90.40	108.94
7	h	501	ANP	O5'-PA-O1A	-4.68	90.40	108.94
7	d	501	ANP	O5'-PA-O1A	-4.68	90.40	108.94
7	a	501	ANP	O5'-PA-O1A	-4.66	90.45	108.94
7	f	501	ANP	O5'-PA-O1A	-4.66	90.46	108.94
7	K	501	ANP	O5'-PA-O1A	-4.66	90.48	108.94
7	c	501	ANP	O5'-PA-O1A	-4.65	90.49	108.94
7	e	501	ANP	O5'-PA-O1A	-4.65	90.50	108.94
6	H	501	G2P	N9-C4-N3	4.26	134.47	125.95
6	O	501	G2P	N9-C4-N3	4.23	134.42	125.95
6	D	501	G2P	N9-C4-N3	4.23	134.41	125.95
6	Q	501	G2P	N9-C4-N3	4.22	134.40	125.95
6	F	501	G2P	N9-C4-N3	4.22	134.38	125.95
6	B	501	G2P	N9-C4-N3	4.21	134.37	125.95
6	M	501	G2P	N9-C4-N3	4.20	134.36	125.95
6	S	501	G2P	N9-C4-N3	4.19	134.33	125.95
6	J	501	G2P	N9-C4-N3	4.19	134.32	125.95
6	J	501	G2P	O4'-C4'-C3'	-3.98	97.26	105.15
7	f	501	ANP	C2-N3-C4	3.97	121.53	111.83
6	H	501	G2P	O4'-C4'-C3'	-3.97	97.28	105.15
6	M	501	G2P	O4'-C4'-C3'	-3.97	97.28	105.15
7	b	501	ANP	C2-N3-C4	3.97	121.52	111.83
7	c	501	ANP	C2-N3-C4	3.97	121.52	111.83
6	D	501	G2P	O4'-C4'-C3'	-3.96	97.29	105.15
7	h	501	ANP	C2-N3-C4	3.96	121.50	111.83
7	d	501	ANP	C2-N3-C4	3.96	121.50	111.83
6	Q	501	G2P	O4'-C4'-C3'	-3.96	97.30	105.15
7	K	501	ANP	C2-N3-C4	3.96	121.50	111.83
7	e	501	ANP	C2-N3-C4	3.96	121.49	111.83
6	O	501	G2P	O4'-C4'-C3'	-3.96	97.30	105.15
6	B	501	G2P	O4'-C4'-C3'	-3.96	97.30	105.15
6	F	501	G2P	O4'-C4'-C3'	-3.95	97.31	105.15
6	S	501	G2P	O4'-C4'-C3'	-3.95	97.31	105.15
7	g	501	ANP	C2-N3-C4	3.94	121.47	111.83
7	a	501	ANP	C2-N3-C4	3.93	121.44	111.83
4	G	501	GTP	N9-C4-N3	3.83	133.62	125.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	501	GTP	N9-C4-N3	3.82	133.59	125.95
4	I	501	GTP	N9-C4-N3	3.82	133.58	125.95
4	N	501	GTP	N9-C4-N3	3.79	133.54	125.95
4	P	501	GTP	N9-C4-N3	3.79	133.53	125.95
4	L	501	GTP	N9-C4-N3	3.78	133.51	125.95
4	E	501	GTP	N9-C4-N3	3.78	133.51	125.95
4	A	501	GTP	N9-C4-N3	3.78	133.50	125.95
4	L	501	GTP	C6-C5-N7	3.77	137.16	130.29
4	R	501	GTP	N9-C4-N3	3.77	133.50	125.95
4	R	501	GTP	C6-C5-N7	3.77	137.15	130.29
4	N	501	GTP	C6-C5-N7	3.76	137.13	130.29
4	I	501	GTP	C6-C5-N7	3.76	137.13	130.29
4	C	501	GTP	C6-C5-N7	3.76	137.13	130.29
4	G	501	GTP	C6-C5-N7	3.73	137.07	130.29
7	f	501	ANP	C5-N7-C8	3.73	109.31	103.45
4	A	501	GTP	C6-C5-N7	3.72	137.05	130.29
7	b	501	ANP	C5-N7-C8	3.71	109.28	103.45
4	P	501	GTP	C6-C5-N7	3.70	137.03	130.29
7	g	501	ANP	C5-N7-C8	3.70	109.27	103.45
4	E	501	GTP	C6-C5-N7	3.69	137.01	130.29
7	h	501	ANP	C5-N7-C8	3.69	109.25	103.45
7	d	501	ANP	C5-N7-C8	3.68	109.24	103.45
7	e	501	ANP	C5-N7-C8	3.68	109.23	103.45
7	c	501	ANP	C5-N7-C8	3.67	109.22	103.45
7	a	501	ANP	C5-N7-C8	3.67	109.22	103.45
7	K	501	ANP	C5-N7-C8	3.66	109.21	103.45
6	D	501	G2P	C6-C5-N7	3.58	136.81	130.29
6	B	501	G2P	C6-C5-N7	3.58	136.80	130.29
6	J	501	G2P	C6-C5-N7	3.57	136.79	130.29
6	M	501	G2P	C6-C5-N7	3.57	136.79	130.29
6	O	501	G2P	C6-C5-N7	3.56	136.78	130.29
6	S	501	G2P	C6-C5-N7	3.56	136.77	130.29
6	H	501	G2P	C6-C5-N7	3.55	136.75	130.29
6	F	501	G2P	C6-C5-N7	3.55	136.75	130.29
6	Q	501	G2P	C6-C5-N7	3.52	136.70	130.29
7	f	501	ANP	N9-C8-N7	-3.46	109.02	113.94
7	h	501	ANP	O2B-PB-O3A	3.45	116.15	104.64
7	f	501	ANP	O2B-PB-O3A	3.44	116.14	104.64
7	K	501	ANP	O2B-PB-O3A	3.44	116.12	104.64
7	a	501	ANP	O2B-PB-O3A	3.44	116.11	104.64
7	c	501	ANP	O2B-PB-O3A	3.43	116.10	104.64
7	b	501	ANP	O2B-PB-O3A	3.43	116.08	104.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	e	501	ANP	O2B-PB-O3A	3.43	116.08	104.64
7	d	501	ANP	N9-C8-N7	-3.42	109.08	113.94
7	g	501	ANP	O2B-PB-O3A	3.42	116.05	104.64
7	h	501	ANP	N9-C8-N7	-3.42	109.09	113.94
6	S	501	G2P	PB-O3B-PG	-3.41	120.22	132.45
7	d	501	ANP	O2B-PB-O3A	3.41	116.03	104.64
7	g	501	ANP	N9-C8-N7	-3.41	109.10	113.94
6	J	501	G2P	PB-O3B-PG	-3.41	120.24	132.45
6	M	501	G2P	PB-O3B-PG	-3.41	120.25	132.45
6	Q	501	G2P	PB-O3B-PG	-3.40	120.26	132.45
7	b	501	ANP	N9-C8-N7	-3.40	109.11	113.94
6	O	501	G2P	PB-O3B-PG	-3.40	120.26	132.45
6	F	501	G2P	PB-O3B-PG	-3.40	120.27	132.45
7	e	501	ANP	N9-C8-N7	-3.40	109.12	113.94
6	H	501	G2P	PB-O3B-PG	-3.39	120.30	132.45
6	B	501	G2P	PB-O3B-PG	-3.39	120.31	132.45
6	D	501	G2P	PB-O3B-PG	-3.39	120.31	132.45
7	c	501	ANP	N9-C8-N7	-3.38	109.14	113.94
7	K	501	ANP	N9-C8-N7	-3.37	109.16	113.94
7	a	501	ANP	N9-C8-N7	-3.37	109.16	113.94
6	D	501	G2P	O2'-C2'-C3'	-3.15	101.73	111.82
6	F	501	G2P	O2'-C2'-C3'	-3.14	101.76	111.82
6	O	501	G2P	O2'-C2'-C3'	-3.14	101.76	111.82
6	M	501	G2P	O2'-C2'-C3'	-3.13	101.78	111.82
6	H	501	G2P	O2'-C2'-C3'	-3.13	101.80	111.82
6	B	501	G2P	O2'-C2'-C3'	-3.13	101.80	111.82
6	S	501	G2P	O2'-C2'-C3'	-3.12	101.80	111.82
6	B	501	G2P	C4-C5-N7	-3.12	105.72	110.67
6	Q	501	G2P	O2'-C2'-C3'	-3.12	101.81	111.82
6	J	501	G2P	O2'-C2'-C3'	-3.12	101.83	111.82
7	K	501	ANP	PA-O5'-C5'	-3.11	103.51	121.35
7	b	501	ANP	PA-O5'-C5'	-3.11	103.52	121.35
7	d	501	ANP	PA-O5'-C5'	-3.11	103.53	121.35
7	f	501	ANP	PA-O5'-C5'	-3.11	103.53	121.35
7	a	501	ANP	PA-O5'-C5'	-3.11	103.53	121.35
7	g	501	ANP	PA-O5'-C5'	-3.11	103.53	121.35
7	c	501	ANP	PA-O5'-C5'	-3.11	103.54	121.35
7	e	501	ANP	PA-O5'-C5'	-3.11	103.55	121.35
6	F	501	G2P	C4-C5-N7	-3.11	105.75	110.67
6	J	501	G2P	C4-C5-N7	-3.10	105.75	110.67
6	D	501	G2P	C4-C5-N7	-3.10	105.76	110.67
7	h	501	ANP	PA-O5'-C5'	-3.10	103.61	121.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	501	G2P	C4-C5-N7	-3.09	105.77	110.67
6	S	501	G2P	C4-C5-N7	-3.09	105.77	110.67
4	N	501	GTP	C4-C5-N7	-3.08	105.79	110.67
6	M	501	G2P	C4-C5-N7	-3.08	105.79	110.67
4	C	501	GTP	C4-C5-N7	-3.07	105.80	110.67
6	O	501	G2P	C4-C5-N7	-3.07	105.80	110.67
6	Q	501	G2P	C4-C5-N7	-3.06	105.82	110.67
4	R	501	GTP	C4-C5-N7	-3.06	105.82	110.67
4	L	501	GTP	C4-C5-N7	-3.05	105.83	110.67
4	I	501	GTP	C4-C5-N7	-3.05	105.83	110.67
4	A	501	GTP	C4-C5-N7	-3.05	105.83	110.67
4	E	501	GTP	C4-C5-N7	-3.04	105.86	110.67
4	G	501	GTP	C4-C5-N7	-3.03	105.87	110.67
4	P	501	GTP	C4-C5-N7	-3.03	105.87	110.67
6	B	501	G2P	O2'-C2'-C1'	3.02	120.49	110.10
6	M	501	G2P	O2'-C2'-C1'	3.02	120.49	110.10
6	S	501	G2P	O2'-C2'-C1'	3.01	120.48	110.10
6	H	501	G2P	O2'-C2'-C1'	3.01	120.48	110.10
6	Q	501	G2P	O2'-C2'-C1'	3.01	120.48	110.10
6	J	501	G2P	O2'-C2'-C1'	3.01	120.47	110.10
6	S	501	G2P	O1B-PB-O2B	3.01	119.73	109.95
6	O	501	G2P	O2'-C2'-C1'	3.01	120.45	110.10
6	F	501	G2P	O2'-C2'-C1'	3.00	120.45	110.10
6	D	501	G2P	O2'-C2'-C1'	3.00	120.44	110.10
6	O	501	G2P	O1B-PB-O2B	3.00	119.72	109.95
6	B	501	G2P	O1B-PB-O2B	3.00	119.70	109.95
6	Q	501	G2P	O1B-PB-O2B	2.99	119.69	109.95
6	D	501	G2P	O1B-PB-O2B	2.99	119.68	109.95
6	F	501	G2P	O1B-PB-O2B	2.99	119.67	109.95
6	H	501	G2P	O1B-PB-O2B	2.98	119.66	109.95
6	J	501	G2P	O1B-PB-O2B	2.98	119.66	109.95
6	M	501	G2P	O1B-PB-O2B	2.97	119.62	109.95
7	a	501	ANP	C2'-C1'-N9	-2.77	106.41	113.30
7	c	501	ANP	C2'-C1'-N9	-2.77	106.41	113.30
7	K	501	ANP	C2'-C1'-N9	-2.77	106.42	113.30
7	f	501	ANP	C2'-C1'-N9	-2.76	106.44	113.30
7	e	501	ANP	C2'-C1'-N9	-2.76	106.44	113.30
7	d	501	ANP	C2'-C1'-N9	-2.76	106.44	113.30
7	h	501	ANP	C2'-C1'-N9	-2.76	106.44	113.30
7	b	501	ANP	C2'-C1'-N9	-2.75	106.46	113.30
7	g	501	ANP	C2'-C1'-N9	-2.74	106.50	113.30
7	e	501	ANP	O2A-PA-O1A	2.72	125.09	112.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	a	501	ANP	O2A-PA-O1A	2.71	125.06	112.44
7	b	501	ANP	O2A-PA-O1A	2.71	125.05	112.44
7	g	501	ANP	O2A-PA-O1A	2.71	125.05	112.44
7	f	501	ANP	O2A-PA-O1A	2.71	125.04	112.44
7	c	501	ANP	O2A-PA-O1A	2.71	125.04	112.44
7	d	501	ANP	O2A-PA-O1A	2.70	125.02	112.44
7	b	501	ANP	O1G-PG-N3B	2.70	115.74	111.77
7	K	501	ANP	O2A-PA-O1A	2.70	125.00	112.44
7	h	501	ANP	O2A-PA-O1A	2.69	124.98	112.44
7	h	501	ANP	O1G-PG-N3B	2.69	115.74	111.77
7	a	501	ANP	O4'-C4'-C5'	-2.69	100.72	109.33
7	g	501	ANP	O4'-C4'-C5'	-2.69	100.72	109.33
6	B	501	G2P	C3'-C2'-C1'	-2.69	96.38	101.46
6	O	501	G2P	C3'-C2'-C1'	-2.69	96.38	101.46
7	c	501	ANP	O4'-C4'-C5'	-2.68	100.73	109.33
6	J	501	G2P	C3'-C2'-C1'	-2.68	96.38	101.46
7	c	501	ANP	O1G-PG-N3B	2.68	115.72	111.77
7	a	501	ANP	O1G-PG-N3B	2.68	115.72	111.77
7	K	501	ANP	O1G-PG-N3B	2.68	115.71	111.77
7	d	501	ANP	O1G-PG-N3B	2.68	115.71	111.77
7	K	501	ANP	O4'-C4'-C5'	-2.68	100.76	109.33
7	e	501	ANP	O4'-C4'-C5'	-2.67	100.77	109.33
7	g	501	ANP	O1G-PG-N3B	2.67	115.71	111.77
6	Q	501	G2P	C3'-C2'-C1'	-2.67	96.41	101.46
6	S	501	G2P	C3'-C2'-C1'	-2.67	96.41	101.46
6	D	501	G2P	C3'-C2'-C1'	-2.67	96.42	101.46
6	M	501	G2P	C3'-C2'-C1'	-2.67	96.42	101.46
7	f	501	ANP	O4'-C4'-C5'	-2.66	100.80	109.33
6	H	501	G2P	C3'-C2'-C1'	-2.66	96.42	101.46
7	h	501	ANP	O4'-C4'-C5'	-2.66	100.81	109.33
7	f	501	ANP	O1G-PG-N3B	2.66	115.69	111.77
7	e	501	ANP	O1G-PG-N3B	2.66	115.68	111.77
7	d	501	ANP	O4'-C4'-C5'	-2.65	100.84	109.33
7	b	501	ANP	O4'-C4'-C5'	-2.65	100.86	109.33
6	F	501	G2P	C3'-C2'-C1'	-2.64	96.47	101.46
7	d	501	ANP	C2'-C3'-C4'	2.62	107.66	102.61
7	c	501	ANP	C2'-C3'-C4'	2.60	107.63	102.61
7	K	501	ANP	C2'-C3'-C4'	2.60	107.62	102.61
7	g	501	ANP	C2'-C3'-C4'	2.59	107.62	102.61
7	f	501	ANP	C2'-C3'-C4'	2.59	107.61	102.61
7	b	501	ANP	C2'-C3'-C4'	2.59	107.60	102.61
7	e	501	ANP	C2'-C3'-C4'	2.58	107.59	102.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	a	501	ANP	C2'-C3'-C4'	2.57	107.58	102.61
7	h	501	ANP	C2'-C3'-C4'	2.57	107.57	102.61
6	O	501	G2P	O5'-C5'-C4'	-2.43	100.72	108.99
6	J	501	G2P	O5'-C5'-C4'	-2.43	100.72	108.99
7	f	501	ANP	C4-N9-C8	2.42	108.28	105.74
6	D	501	G2P	O5'-C5'-C4'	-2.42	100.75	108.99
6	S	501	G2P	O5'-C5'-C4'	-2.42	100.76	108.99
6	H	501	G2P	O5'-C5'-C4'	-2.42	100.77	108.99
6	M	501	G2P	O5'-C5'-C4'	-2.41	100.78	108.99
6	Q	501	G2P	O5'-C5'-C4'	-2.41	100.79	108.99
6	B	501	G2P	O5'-C5'-C4'	-2.41	100.79	108.99
6	F	501	G2P	O5'-C5'-C4'	-2.41	100.79	108.99
7	d	501	ANP	C4-N9-C8	2.37	108.22	105.74
7	K	501	ANP	O2G-PG-O1G	-2.36	107.54	113.45
7	g	501	ANP	C4-N9-C8	2.36	108.21	105.74
7	e	501	ANP	O2G-PG-O1G	-2.35	107.55	113.45
7	g	501	ANP	O2G-PG-O1G	-2.34	107.58	113.45
7	h	501	ANP	O2G-PG-O1G	-2.34	107.58	113.45
7	c	501	ANP	C4-N9-C8	2.34	108.19	105.74
7	c	501	ANP	O2G-PG-O1G	-2.34	107.59	113.45
7	b	501	ANP	C4-N9-C8	2.33	108.19	105.74
7	f	501	ANP	O2G-PG-O1G	-2.33	107.60	113.45
7	a	501	ANP	C4-N9-C8	2.33	108.19	105.74
7	b	501	ANP	O2G-PG-O1G	-2.33	107.61	113.45
7	a	501	ANP	O2G-PG-O1G	-2.33	107.61	113.45
7	h	501	ANP	C4-N9-C8	2.32	108.18	105.74
7	d	501	ANP	O2G-PG-O1G	-2.32	107.62	113.45
7	K	501	ANP	C4-N9-C8	2.32	108.17	105.74
7	e	501	ANP	C4-N9-C8	2.30	108.16	105.74
6	J	501	G2P	C8-N7-C5	2.28	108.32	104.26
6	D	501	G2P	C8-N7-C5	2.28	108.31	104.26
6	F	501	G2P	C8-N7-C5	2.28	108.31	104.26
6	B	501	G2P	C8-N7-C5	2.27	108.31	104.26
6	M	501	G2P	C8-N7-C5	2.26	108.29	104.26
6	Q	501	G2P	C8-N7-C5	2.26	108.29	104.26
6	O	501	G2P	C8-N7-C5	2.25	108.27	104.26
6	S	501	G2P	C8-N7-C5	2.25	108.26	104.26
6	H	501	G2P	C8-N7-C5	2.23	108.23	104.26
4	R	501	GTP	C8-N7-C5	2.17	108.12	104.26
4	I	501	GTP	C8-N7-C5	2.16	108.11	104.26
4	C	501	GTP	C8-N7-C5	2.15	108.08	104.26
4	L	501	GTP	C8-N7-C5	2.14	108.07	104.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	501	GTP	C8-N7-C5	2.14	108.07	104.26
4	R	501	GTP	O6-C6-C5	-2.13	120.91	126.53
4	N	501	GTP	C8-N7-C5	2.12	108.04	104.26
4	P	501	GTP	C8-N7-C5	2.12	108.04	104.26
4	I	501	GTP	O6-C6-C5	-2.12	120.94	126.53
4	G	501	GTP	O6-C6-C5	-2.12	120.94	126.53
4	L	501	GTP	O6-C6-C5	-2.12	120.94	126.53
4	N	501	GTP	O6-C6-C5	-2.12	120.95	126.53
4	C	501	GTP	O6-C6-C5	-2.11	120.96	126.53
4	E	501	GTP	O6-C6-C5	-2.11	120.97	126.53
4	A	501	GTP	C8-N7-C5	2.10	108.01	104.26
4	P	501	GTP	O6-C6-C5	-2.10	120.98	126.53
4	E	501	GTP	C8-N7-C5	2.10	108.01	104.26
4	A	501	GTP	O6-C6-C5	-2.10	121.00	126.53
7	h	501	ANP	O4'-C4'-C3'	2.04	109.21	105.15
6	D	501	G2P	O6-C6-C5	-2.04	121.14	126.53
6	S	501	G2P	O6-C6-C5	-2.04	121.14	126.53
6	F	501	G2P	O6-C6-C5	-2.04	121.14	126.53
7	f	501	ANP	O4'-C4'-C3'	2.04	109.20	105.15
6	B	501	G2P	O6-C6-C5	-2.04	121.15	126.53
7	d	501	ANP	O4'-C4'-C3'	2.04	109.20	105.15
6	O	501	G2P	O6-C6-C5	-2.04	121.15	126.53
7	d	501	ANP	C4-C5-N7	-2.04	108.25	110.58
6	J	501	G2P	O6-C6-C5	-2.03	121.16	126.53
7	c	501	ANP	C4-C5-N7	-2.03	108.26	110.58
7	g	501	ANP	C4-C5-N7	-2.03	108.26	110.58
7	b	501	ANP	O4'-C4'-C3'	2.03	109.19	105.15
7	e	501	ANP	O4'-C4'-C3'	2.03	109.19	105.15
7	K	501	ANP	O4'-C4'-C3'	2.03	109.18	105.15
6	M	501	G2P	O6-C6-C5	-2.02	121.19	126.53
7	K	501	ANP	C4-C5-N7	-2.02	108.27	110.58
7	b	501	ANP	C4-C5-N7	-2.02	108.27	110.58
7	g	501	ANP	O4'-C4'-C3'	2.02	109.16	105.15
7	f	501	ANP	C4-C5-N7	-2.02	108.28	110.58
6	H	501	G2P	O6-C6-C5	-2.02	121.21	126.53
7	c	501	ANP	O4'-C4'-C3'	2.01	109.14	105.15
7	e	501	ANP	C4-C5-N7	-2.01	108.29	110.58
7	a	501	ANP	O4'-C4'-C3'	2.01	109.13	105.15
7	e	501	ANP	C2-N1-C6	2.00	122.02	118.73

There are no chirality outliers.

All (126) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	GTP	PB-O3B-PG-O3G
4	A	501	GTP	C5'-O5'-PA-O3A
4	A	501	GTP	C5'-O5'-PA-O1A
4	A	501	GTP	C5'-O5'-PA-O2A
4	C	501	GTP	PB-O3B-PG-O3G
4	C	501	GTP	C5'-O5'-PA-O3A
4	C	501	GTP	C5'-O5'-PA-O1A
4	C	501	GTP	C5'-O5'-PA-O2A
4	E	501	GTP	PB-O3B-PG-O3G
4	E	501	GTP	C5'-O5'-PA-O3A
4	E	501	GTP	C5'-O5'-PA-O1A
4	E	501	GTP	C5'-O5'-PA-O2A
4	G	501	GTP	PB-O3B-PG-O3G
4	G	501	GTP	C5'-O5'-PA-O3A
4	G	501	GTP	C5'-O5'-PA-O1A
4	G	501	GTP	C5'-O5'-PA-O2A
4	I	501	GTP	PB-O3B-PG-O3G
4	I	501	GTP	C5'-O5'-PA-O3A
4	I	501	GTP	C5'-O5'-PA-O1A
4	I	501	GTP	C5'-O5'-PA-O2A
4	L	501	GTP	PB-O3B-PG-O3G
4	L	501	GTP	C5'-O5'-PA-O3A
4	L	501	GTP	C5'-O5'-PA-O1A
4	L	501	GTP	C5'-O5'-PA-O2A
4	N	501	GTP	PB-O3B-PG-O3G
4	N	501	GTP	C5'-O5'-PA-O3A
4	N	501	GTP	C5'-O5'-PA-O1A
4	N	501	GTP	C5'-O5'-PA-O2A
4	P	501	GTP	PB-O3B-PG-O3G
4	P	501	GTP	C5'-O5'-PA-O3A
4	P	501	GTP	C5'-O5'-PA-O1A
4	P	501	GTP	C5'-O5'-PA-O2A
4	R	501	GTP	PB-O3B-PG-O3G
4	R	501	GTP	C5'-O5'-PA-O3A
4	R	501	GTP	C5'-O5'-PA-O1A
4	R	501	GTP	C5'-O5'-PA-O2A
6	B	501	G2P	PB-O3B-PG-O1G
6	D	501	G2P	PB-O3B-PG-O1G
6	F	501	G2P	PB-O3B-PG-O1G
6	H	501	G2P	PB-O3B-PG-O1G
6	J	501	G2P	PB-O3B-PG-O1G
6	M	501	G2P	PB-O3B-PG-O1G
6	O	501	G2P	PB-O3B-PG-O1G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	Q	501	G2P	PB-O3B-PG-O1G
6	S	501	G2P	PB-O3B-PG-O1G
7	K	501	ANP	PB-N3B-PG-O1G
7	K	501	ANP	PG-N3B-PB-O1B
7	a	501	ANP	PB-N3B-PG-O1G
7	a	501	ANP	PG-N3B-PB-O1B
7	b	501	ANP	PB-N3B-PG-O1G
7	b	501	ANP	PG-N3B-PB-O1B
7	c	501	ANP	PB-N3B-PG-O1G
7	c	501	ANP	PG-N3B-PB-O1B
7	d	501	ANP	PB-N3B-PG-O1G
7	d	501	ANP	PG-N3B-PB-O1B
7	e	501	ANP	PB-N3B-PG-O1G
7	e	501	ANP	PG-N3B-PB-O1B
7	f	501	ANP	PB-N3B-PG-O1G
7	f	501	ANP	PG-N3B-PB-O1B
7	g	501	ANP	PB-N3B-PG-O1G
7	g	501	ANP	PG-N3B-PB-O1B
7	h	501	ANP	PB-N3B-PG-O1G
7	h	501	ANP	PG-N3B-PB-O1B
6	B	501	G2P	C5'-O5'-PA-O1A
6	D	501	G2P	C5'-O5'-PA-O1A
6	F	501	G2P	C5'-O5'-PA-O1A
6	H	501	G2P	C5'-O5'-PA-O1A
6	J	501	G2P	C5'-O5'-PA-O1A
6	M	501	G2P	C5'-O5'-PA-O1A
6	O	501	G2P	C5'-O5'-PA-O1A
6	Q	501	G2P	C5'-O5'-PA-O1A
6	S	501	G2P	C5'-O5'-PA-O1A
6	B	501	G2P	PB-O3B-PG-O2G
6	D	501	G2P	PB-O3B-PG-O2G
6	F	501	G2P	PB-O3B-PG-O2G
6	H	501	G2P	PB-O3B-PG-O2G
6	J	501	G2P	PB-O3B-PG-O2G
6	M	501	G2P	PB-O3B-PG-O2G
6	O	501	G2P	PB-O3B-PG-O2G
6	Q	501	G2P	PB-O3B-PG-O2G
6	S	501	G2P	PB-O3B-PG-O2G
6	B	501	G2P	PB-O3B-PG-O3G
6	D	501	G2P	PB-O3B-PG-O3G
6	F	501	G2P	PB-O3B-PG-O3G
6	H	501	G2P	PB-O3B-PG-O3G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	J	501	G2P	PB-O3B-PG-O3G
6	M	501	G2P	PB-O3B-PG-O3G
6	O	501	G2P	PB-O3B-PG-O3G
6	Q	501	G2P	PB-O3B-PG-O3G
6	S	501	G2P	PB-O3B-PG-O3G
4	A	501	GTP	PB-O3A-PA-O1A
4	A	501	GTP	PB-O3A-PA-O2A
4	C	501	GTP	PB-O3A-PA-O1A
4	C	501	GTP	PB-O3A-PA-O2A
4	E	501	GTP	PB-O3A-PA-O1A
4	E	501	GTP	PB-O3A-PA-O2A
4	G	501	GTP	PB-O3A-PA-O1A
4	G	501	GTP	PB-O3A-PA-O2A
4	I	501	GTP	PB-O3A-PA-O1A
4	I	501	GTP	PB-O3A-PA-O2A
4	L	501	GTP	PB-O3A-PA-O1A
4	N	501	GTP	PB-O3A-PA-O1A
4	N	501	GTP	PB-O3A-PA-O2A
4	P	501	GTP	PB-O3A-PA-O1A
4	P	501	GTP	PB-O3A-PA-O2A
4	R	501	GTP	PB-O3A-PA-O1A
4	R	501	GTP	PB-O3A-PA-O2A
4	A	501	GTP	PB-O3B-PG-O1G
4	C	501	GTP	PB-O3B-PG-O1G
4	E	501	GTP	PB-O3B-PG-O1G
4	G	501	GTP	PB-O3B-PG-O1G
4	I	501	GTP	PB-O3B-PG-O1G
4	L	501	GTP	PB-O3B-PG-O1G
4	N	501	GTP	PB-O3B-PG-O1G
4	P	501	GTP	PB-O3B-PG-O1G
4	R	501	GTP	PB-O3B-PG-O1G
7	K	501	ANP	PG-N3B-PB-O3A
7	a	501	ANP	PG-N3B-PB-O3A
7	b	501	ANP	PG-N3B-PB-O3A
7	c	501	ANP	PG-N3B-PB-O3A
7	d	501	ANP	PG-N3B-PB-O3A
7	e	501	ANP	PG-N3B-PB-O3A
7	f	501	ANP	PG-N3B-PB-O3A
7	g	501	ANP	PG-N3B-PB-O3A
7	h	501	ANP	PG-N3B-PB-O3A
4	L	501	GTP	PB-O3A-PA-O2A

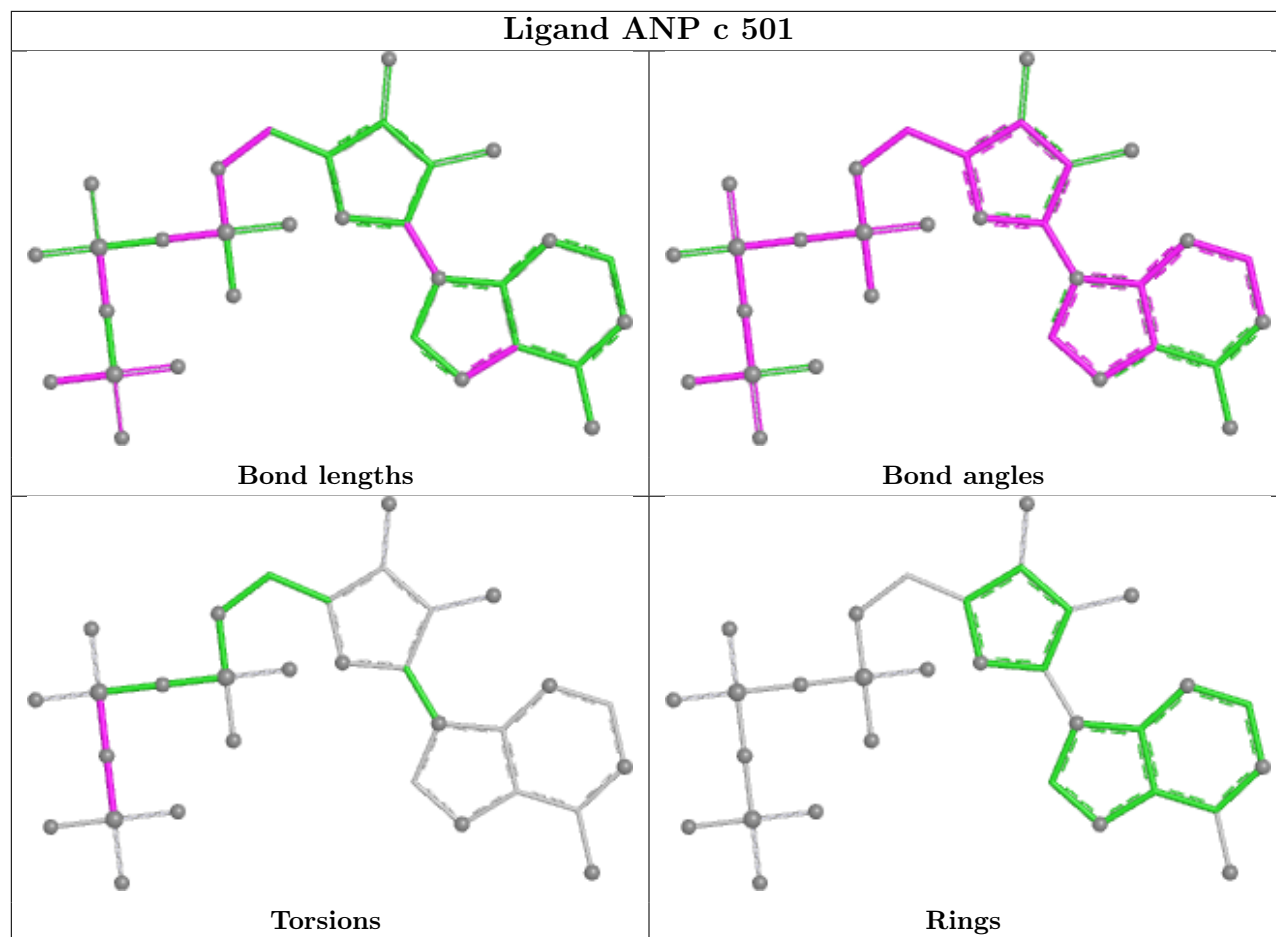
There are no ring outliers.

18 monomers are involved in 31 short contacts:

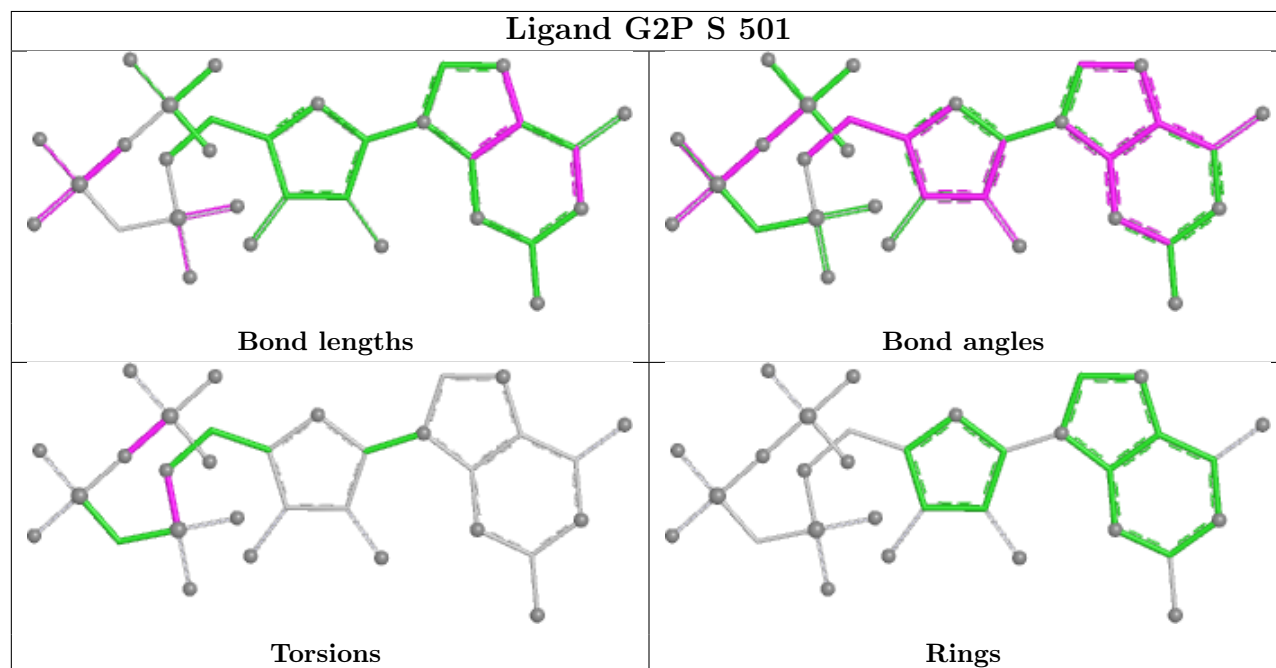
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	c	501	ANP	3	0
6	S	501	G2P	1	0
6	O	501	G2P	1	0
7	b	501	ANP	2	0
6	B	501	G2P	1	0
6	D	501	G2P	1	0
7	e	501	ANP	2	0
6	M	501	G2P	1	0
7	h	501	ANP	2	0
6	F	501	G2P	1	0
6	J	501	G2P	1	0
7	f	501	ANP	3	0
6	Q	501	G2P	1	0
6	H	501	G2P	1	0
7	d	501	ANP	3	0
7	a	501	ANP	2	0
7	K	501	ANP	3	0
7	g	501	ANP	2	0

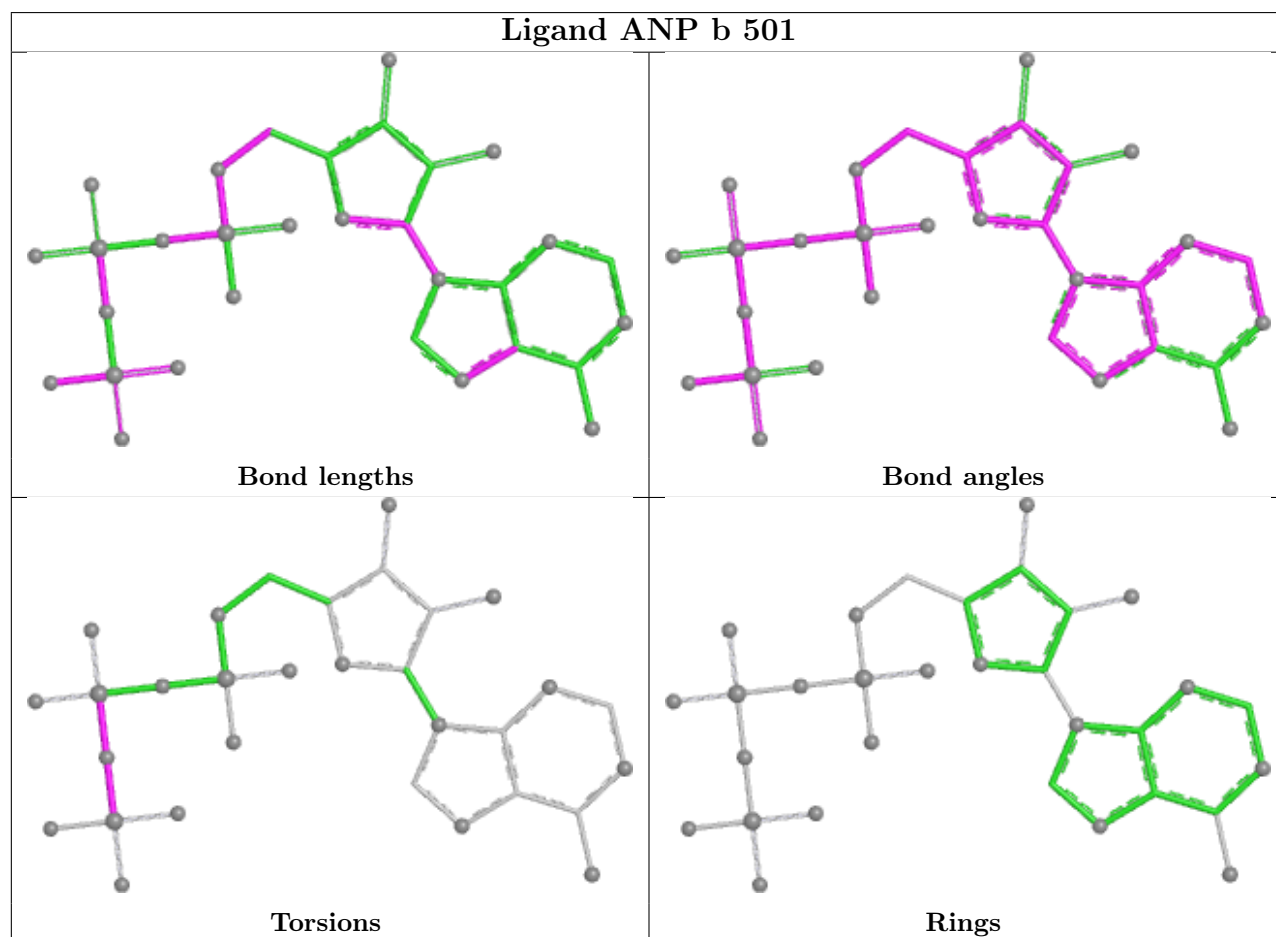
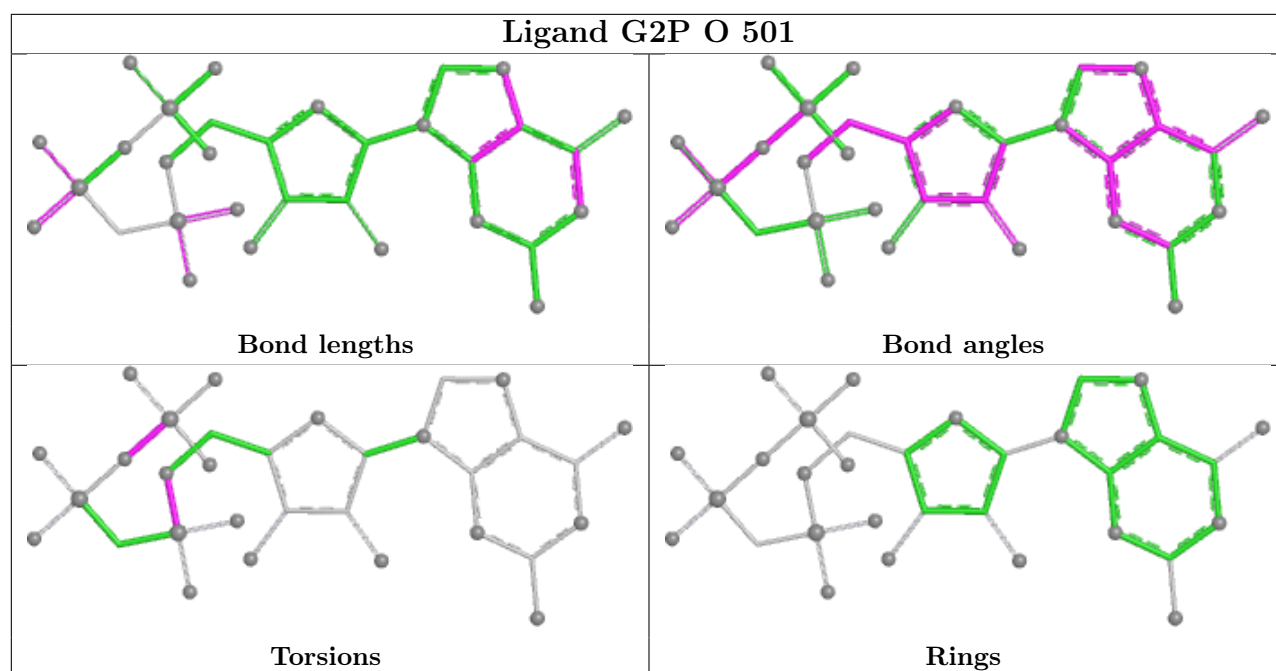
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

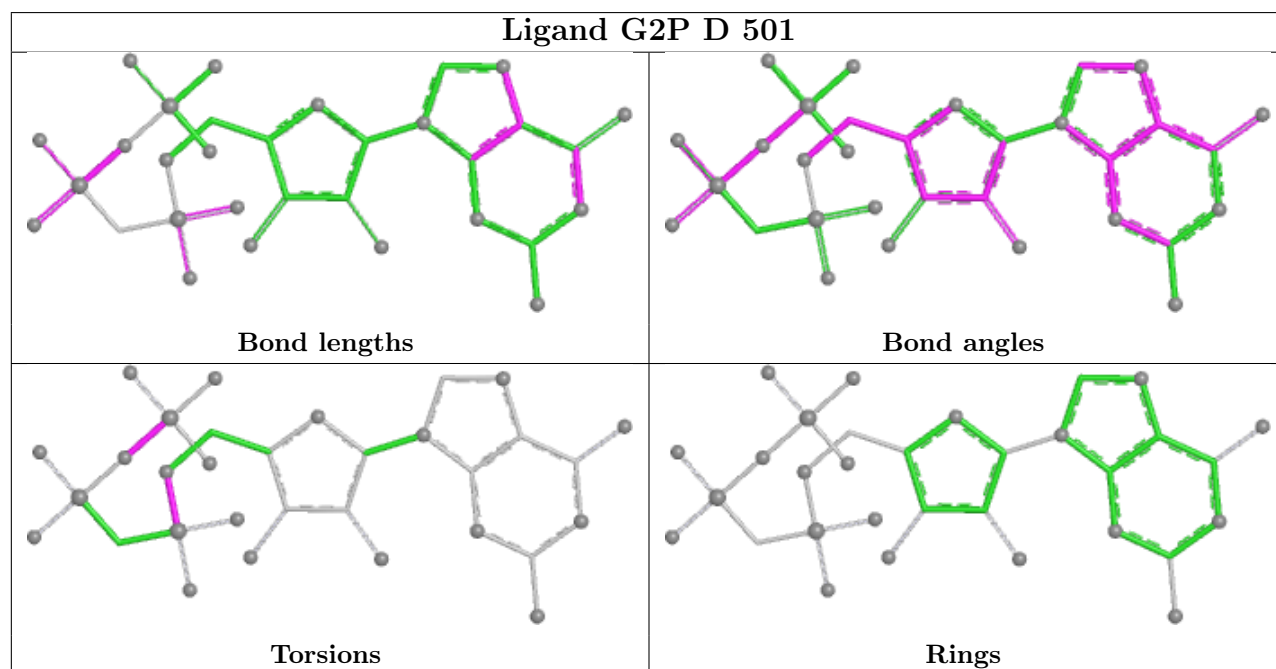
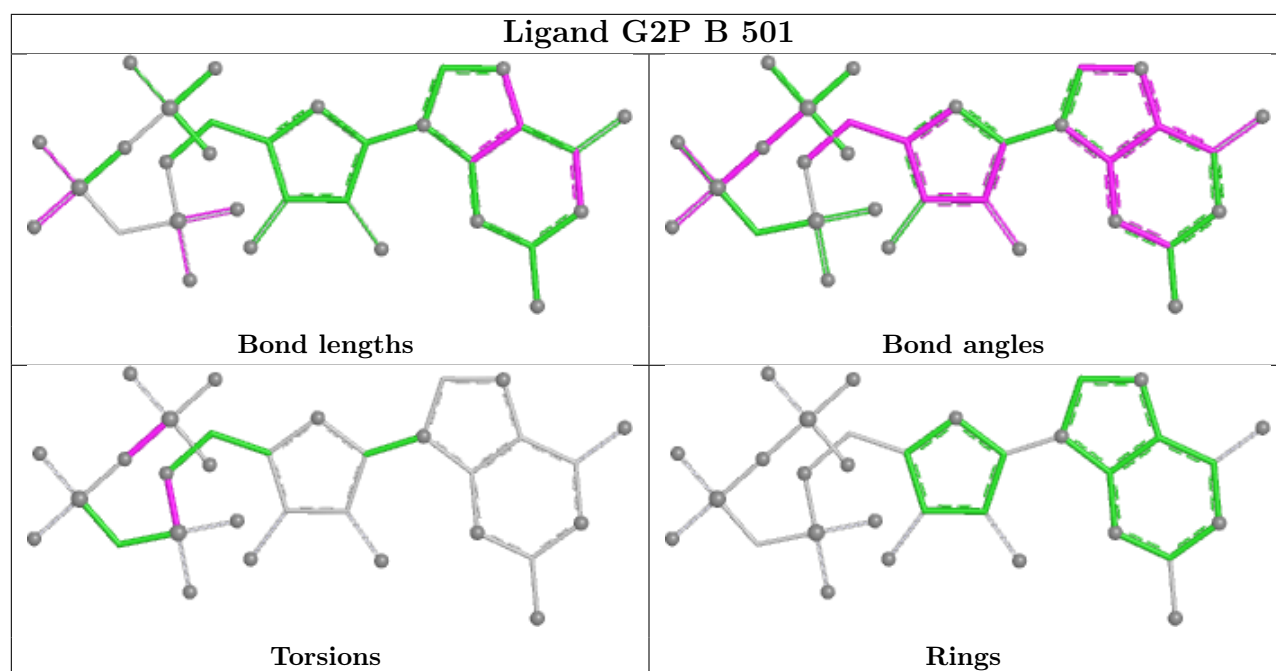
Ligand ANP c 501



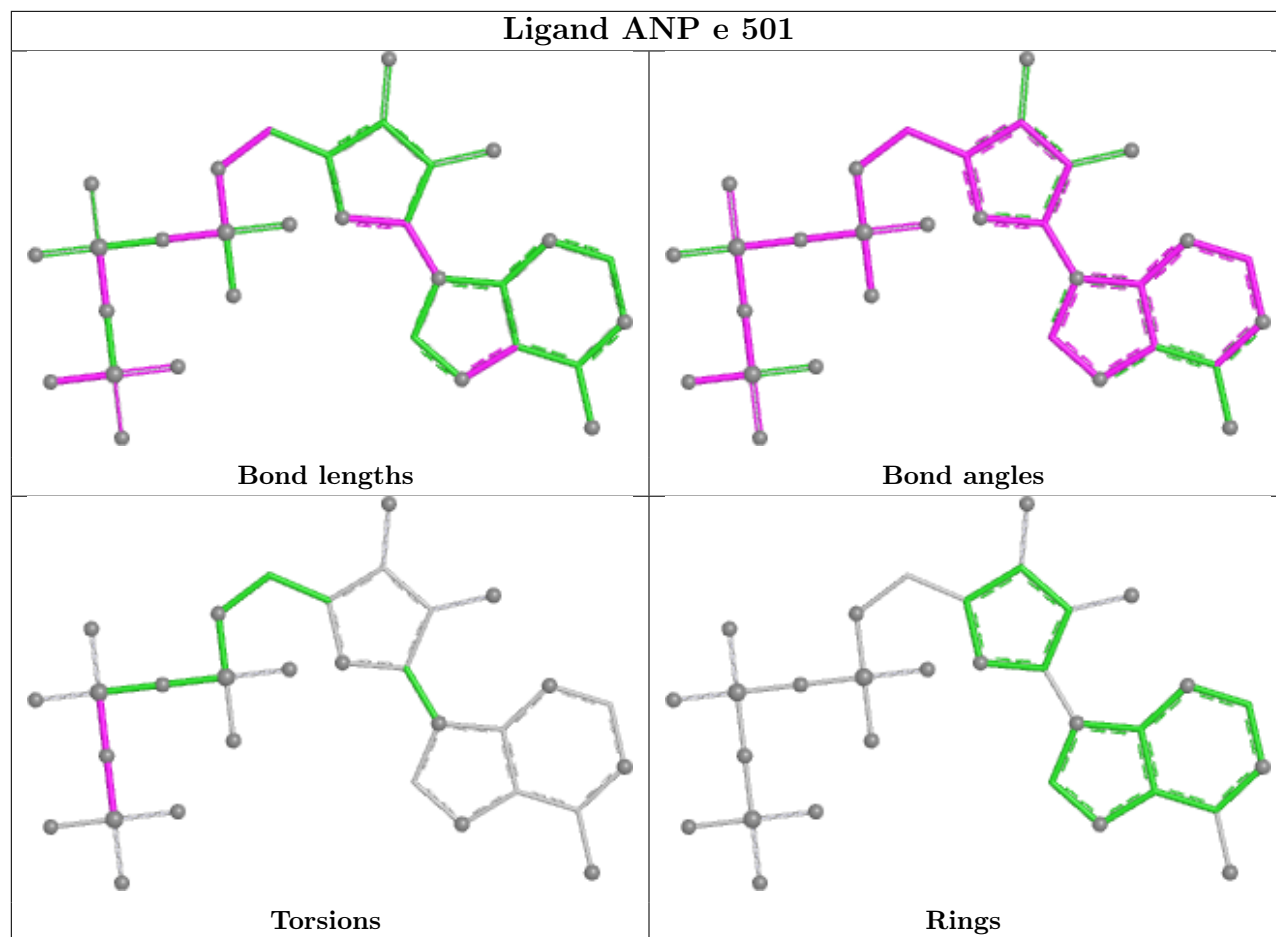
Ligand G2P S 501



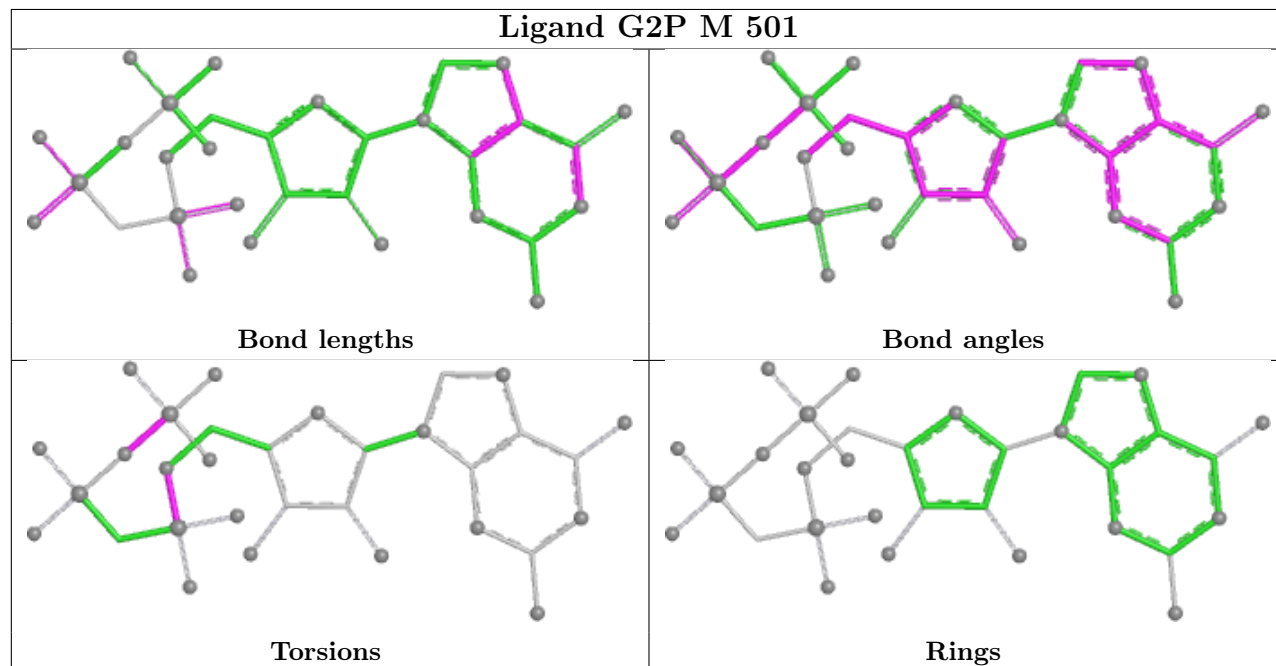




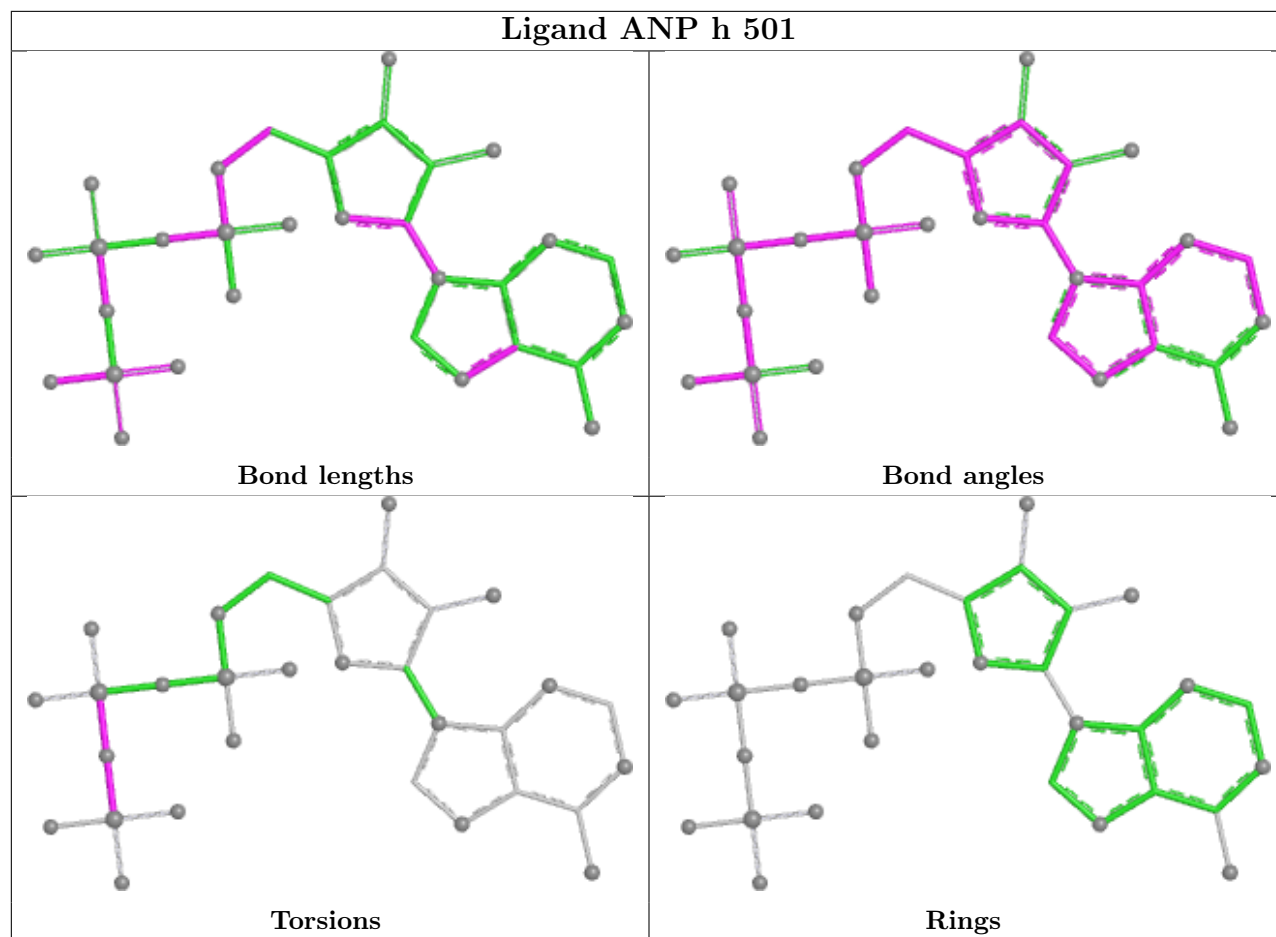
Ligand ANP e 501



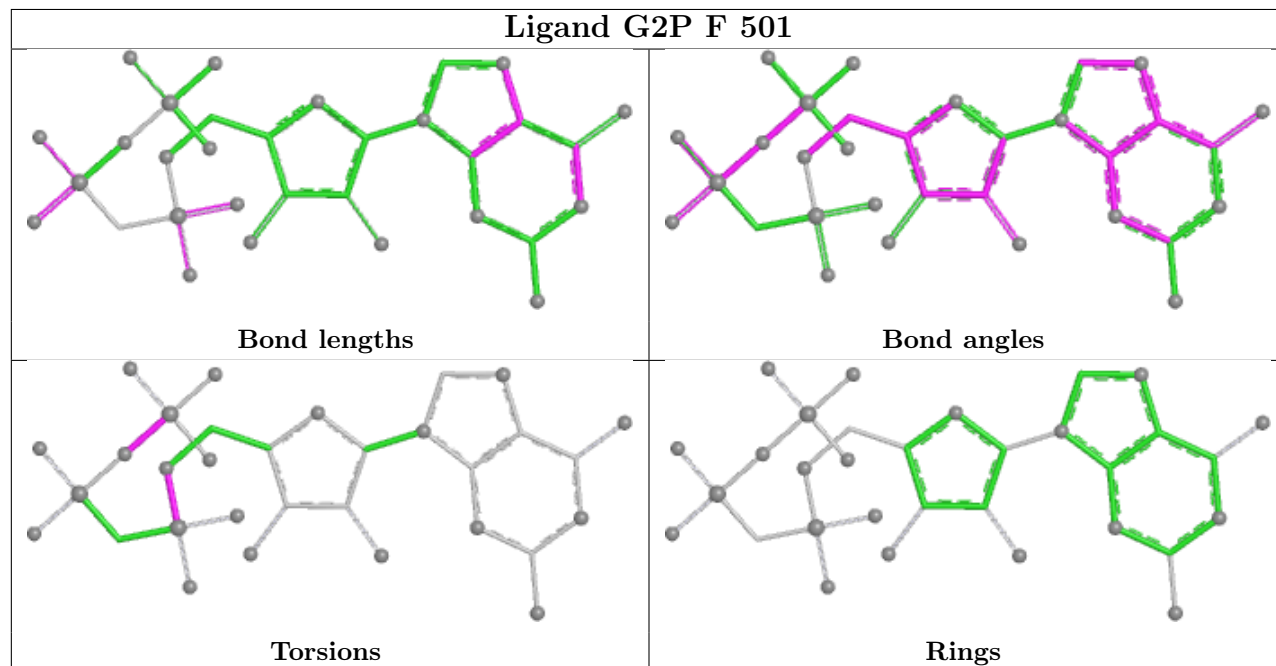
Ligand G2P M 501

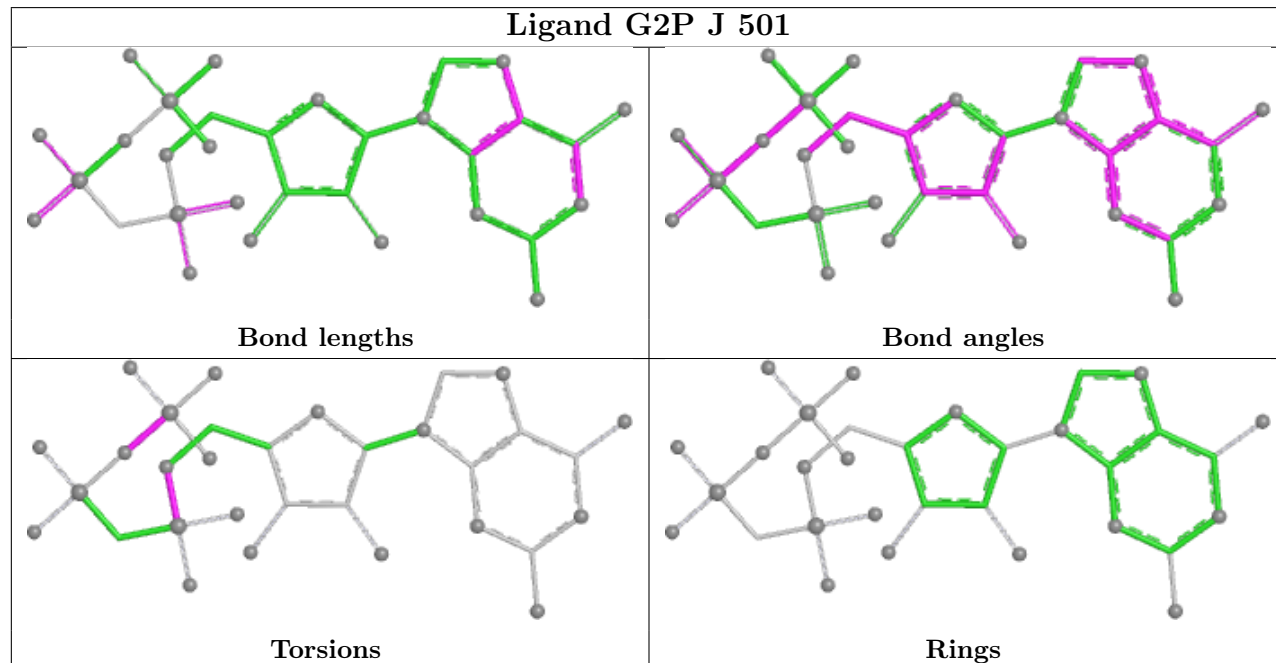
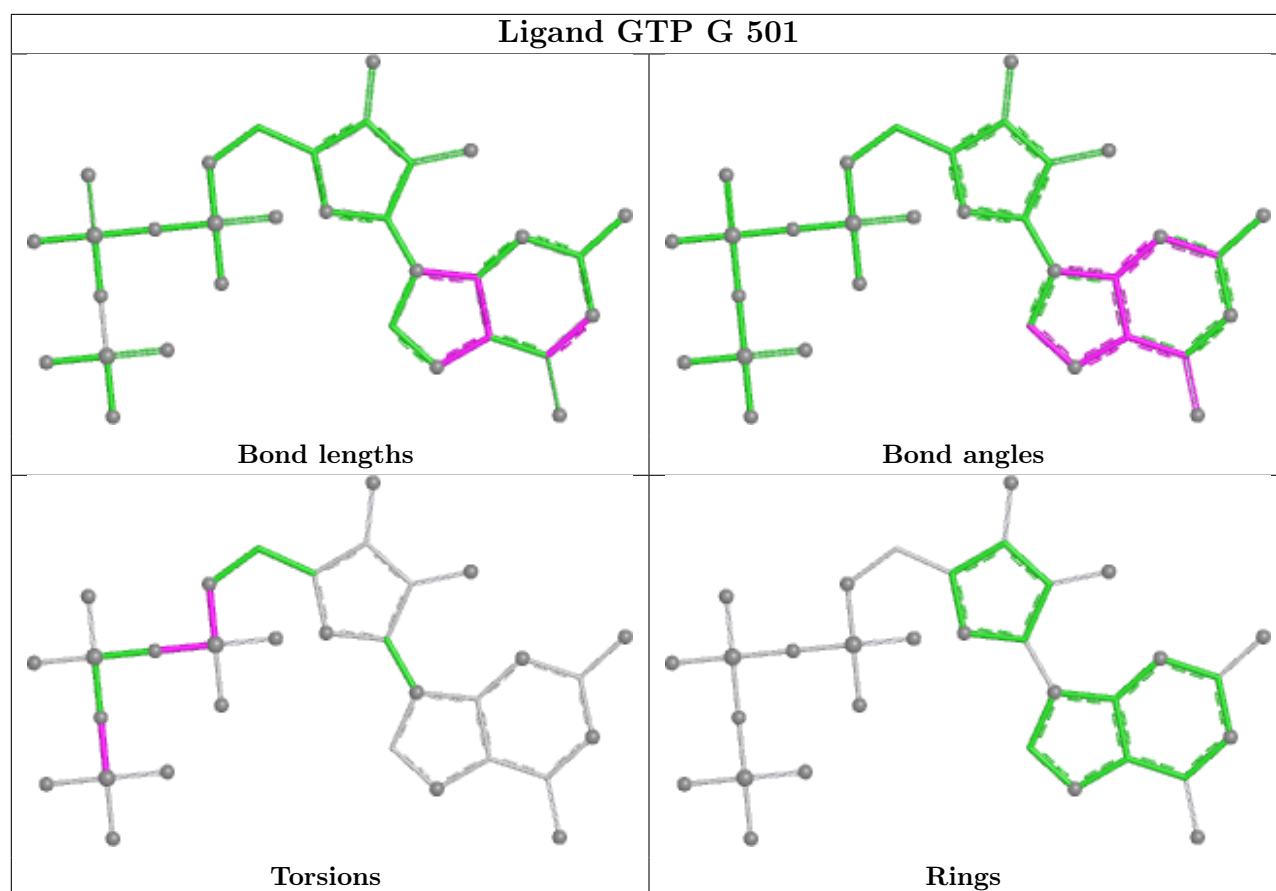


Ligand ANP h 501

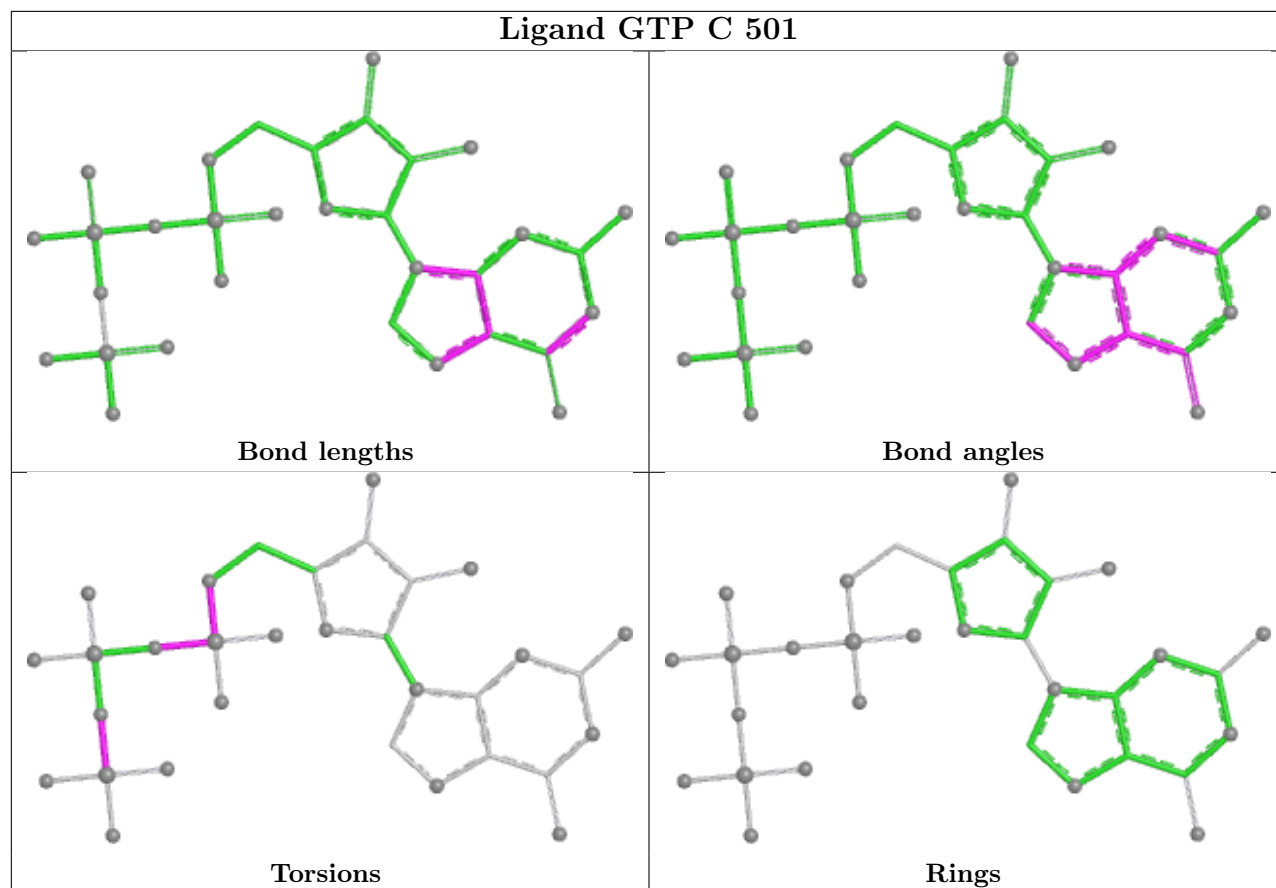


Ligand G2P F 501

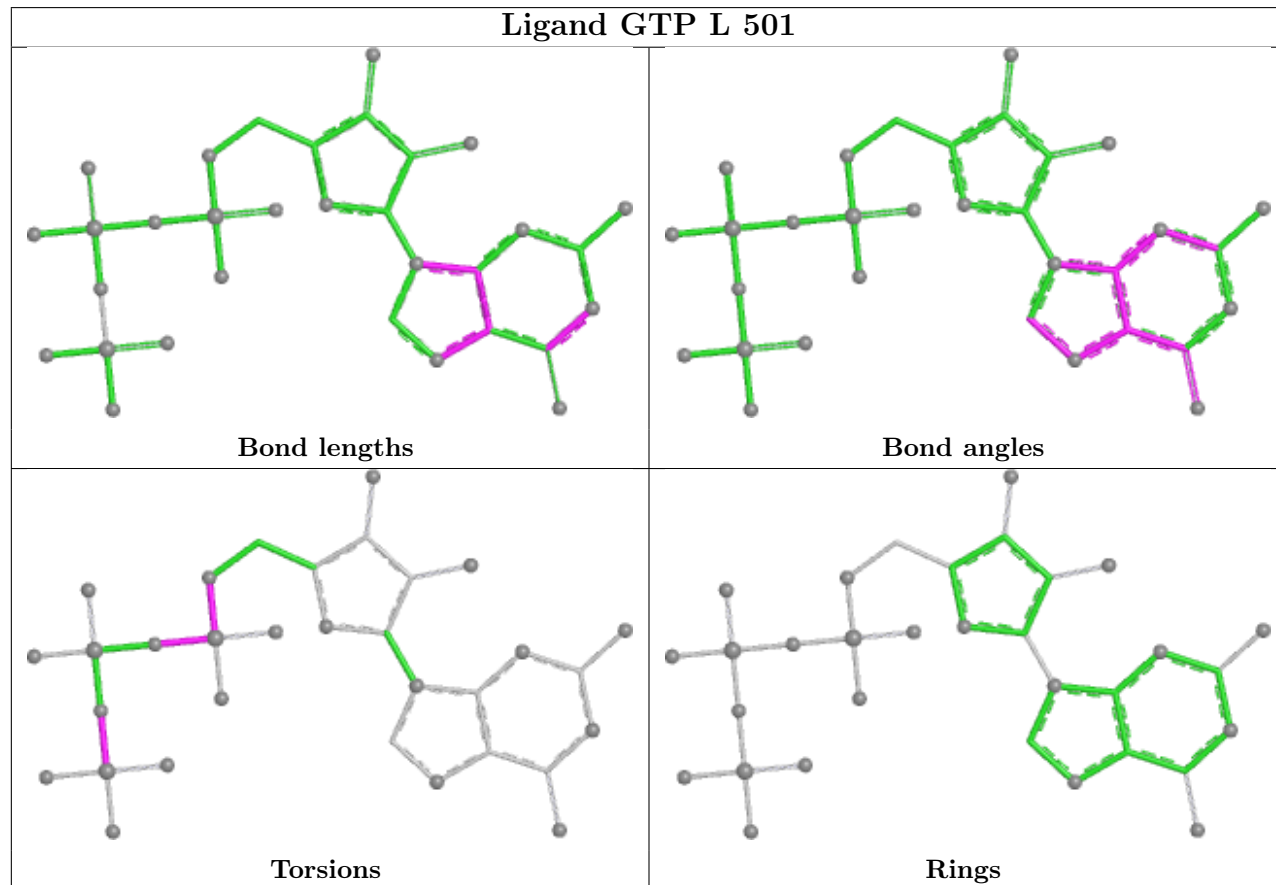




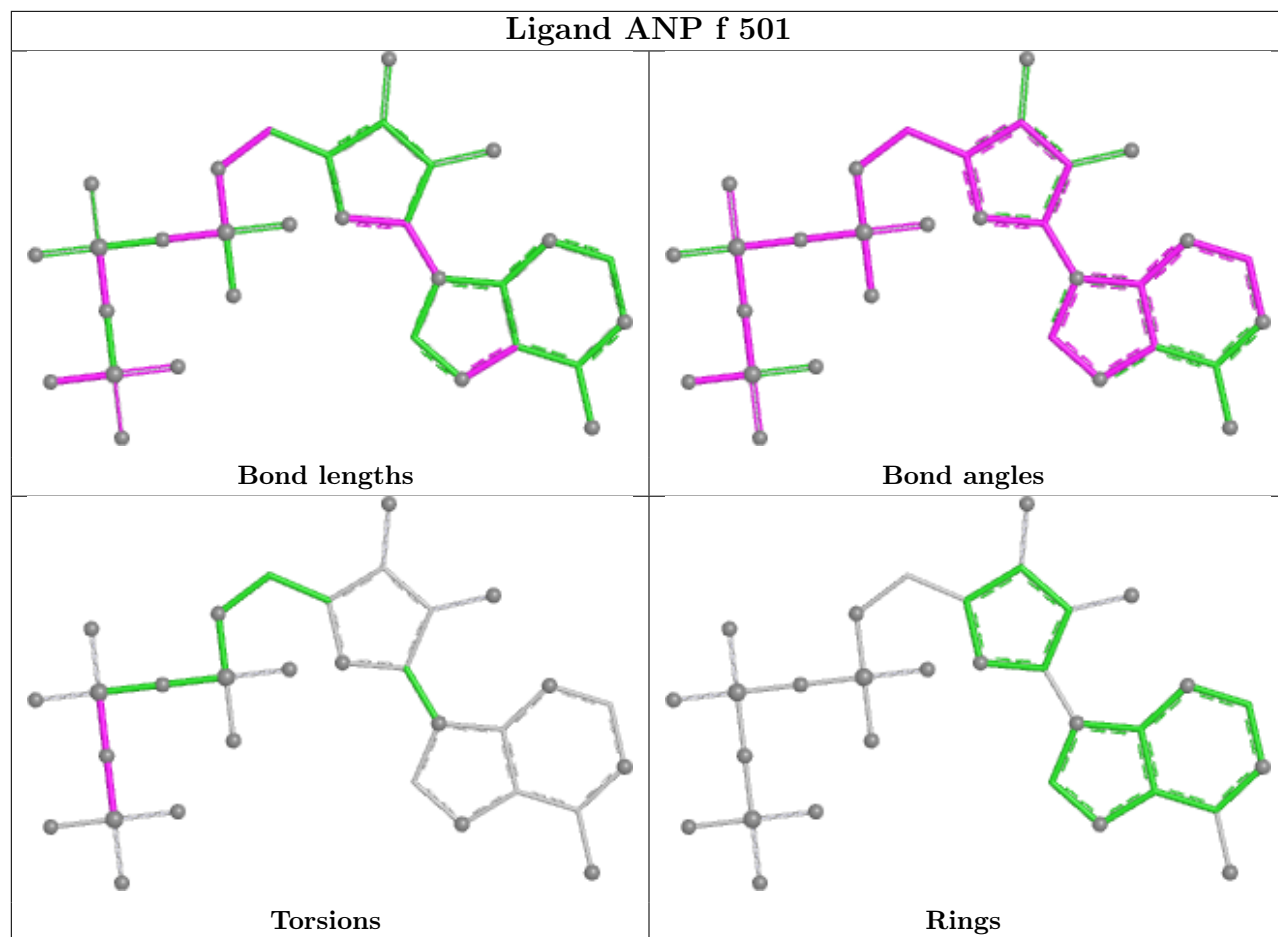
Ligand GTP C 501



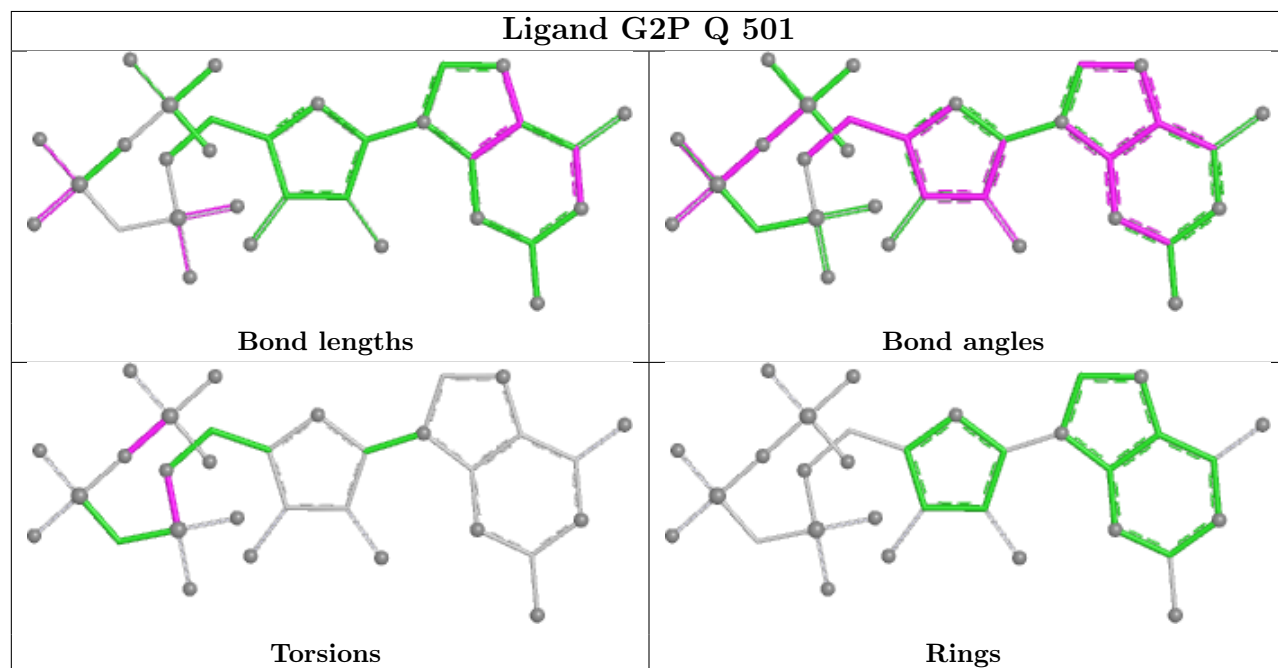
Ligand GTP L 501

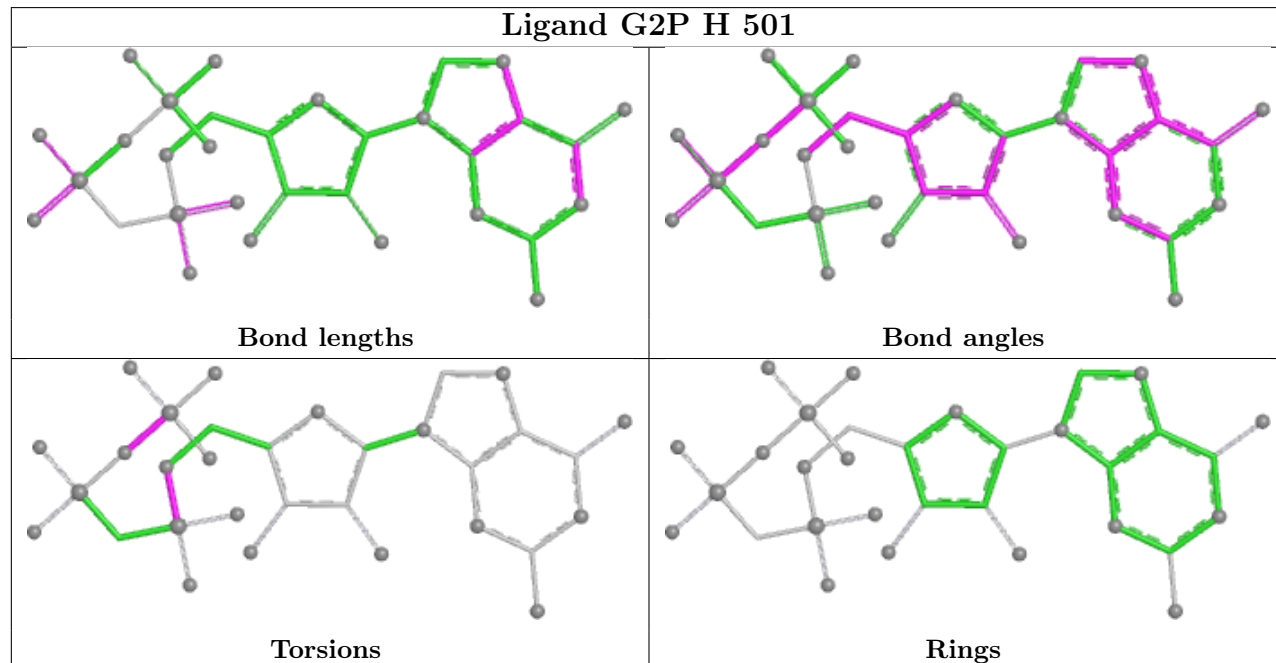
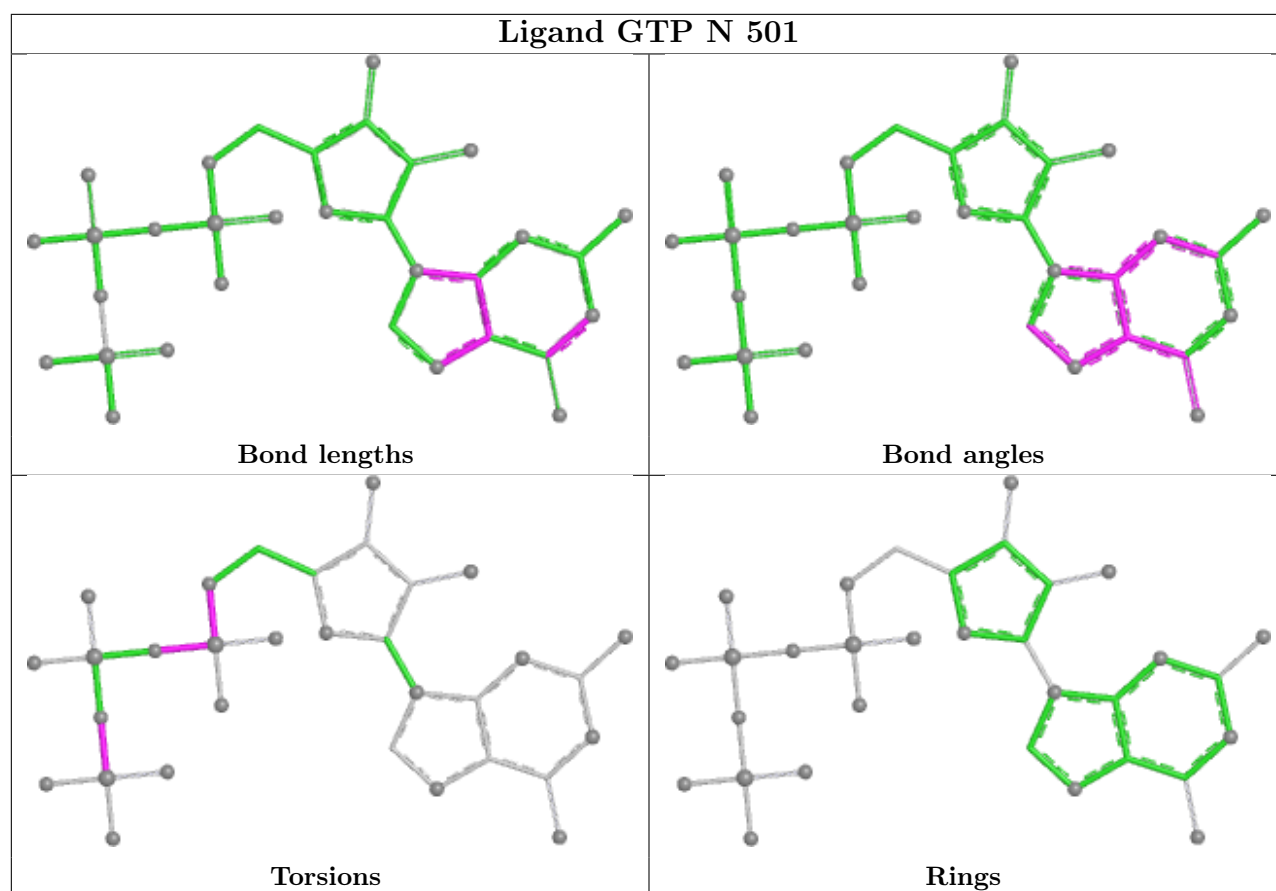


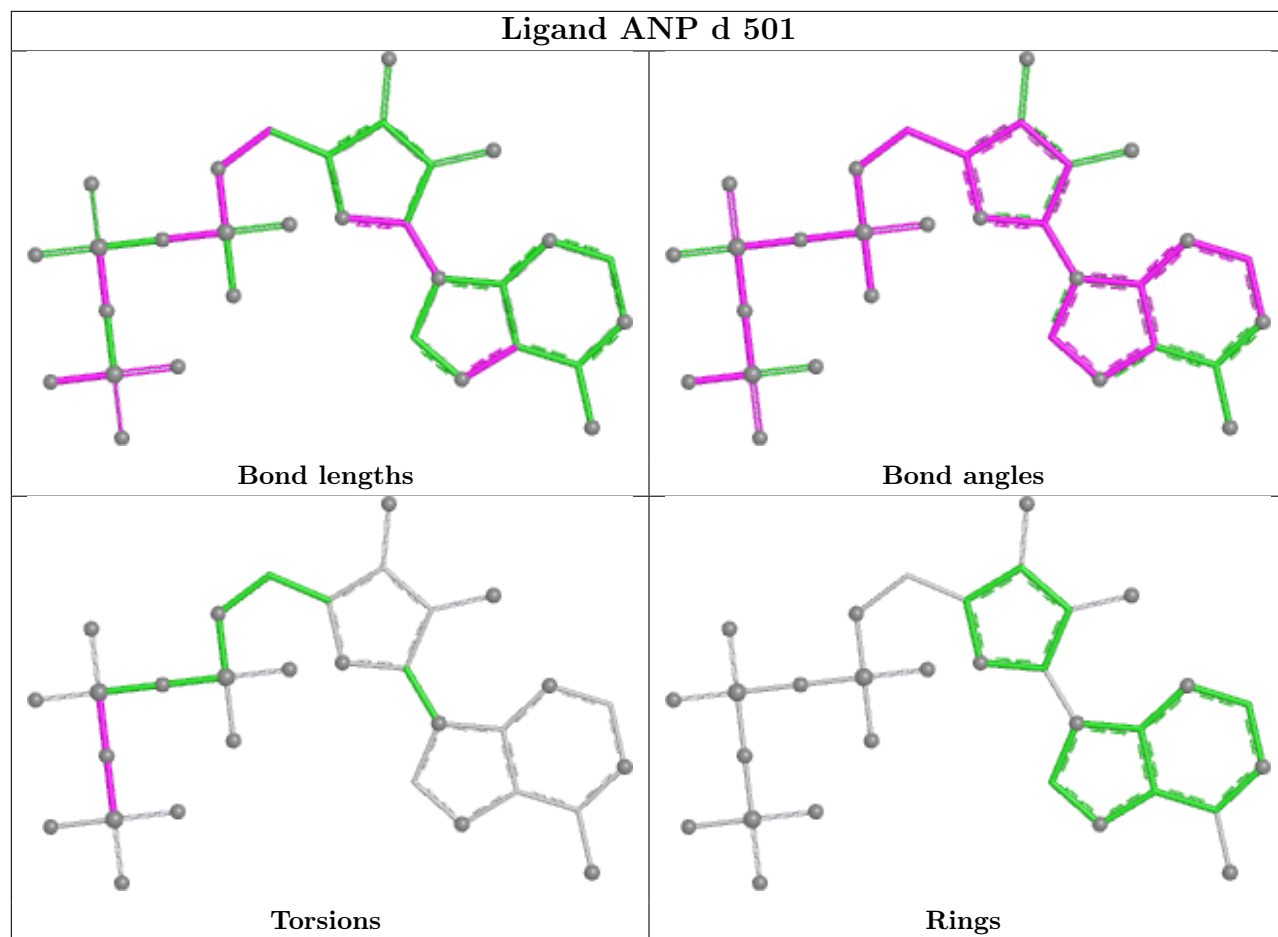
Ligand ANP f 501

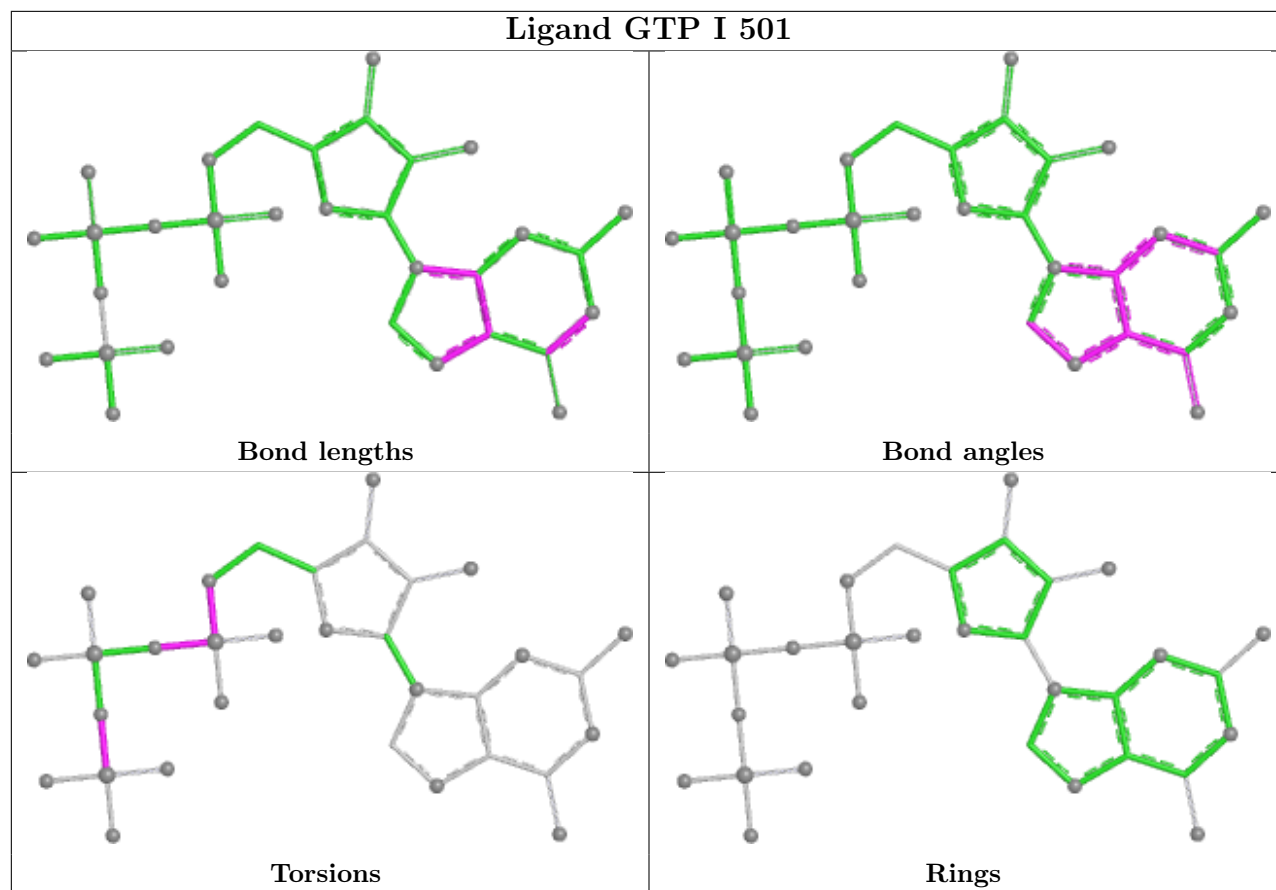


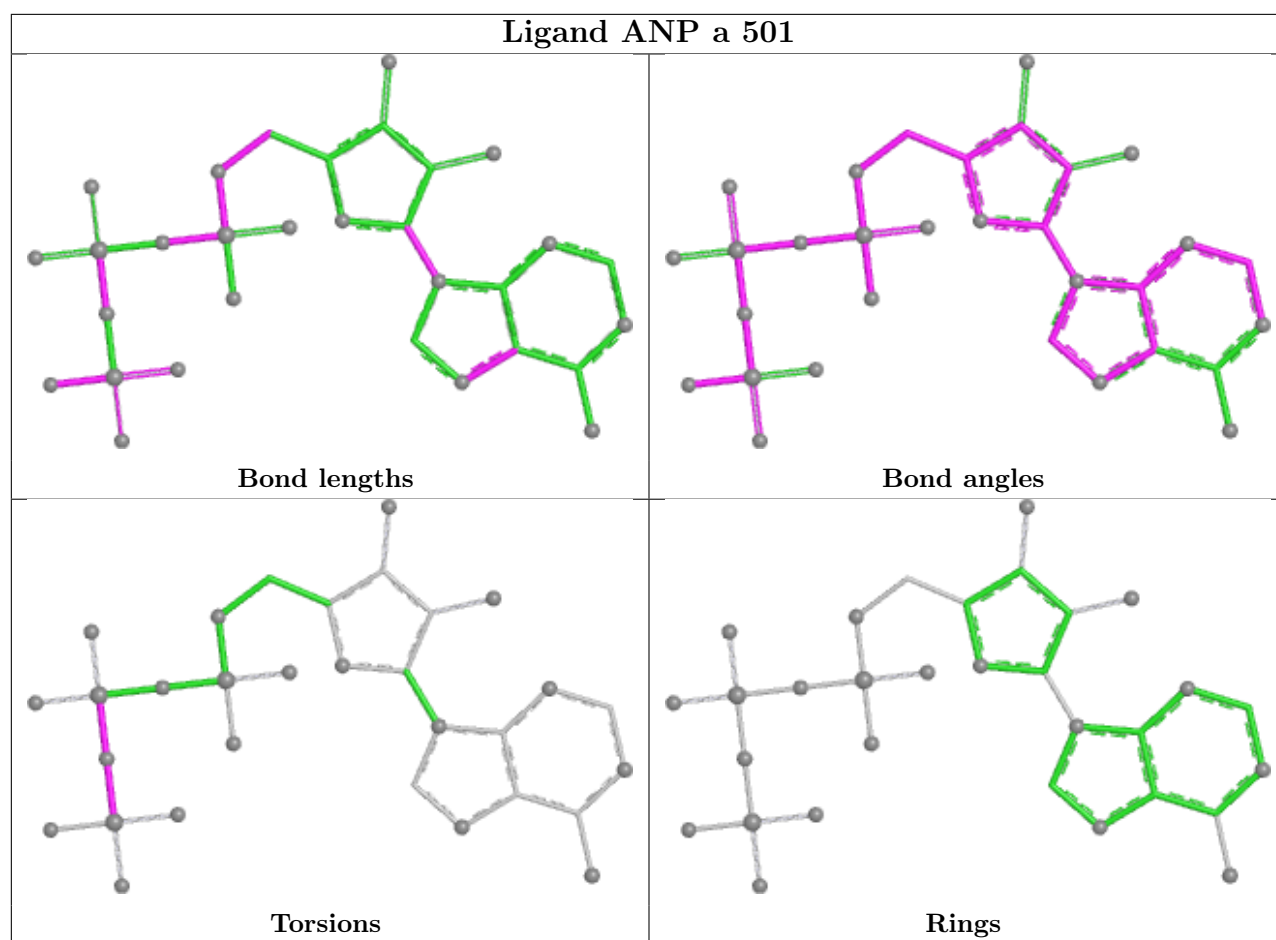
Ligand G2P Q 501

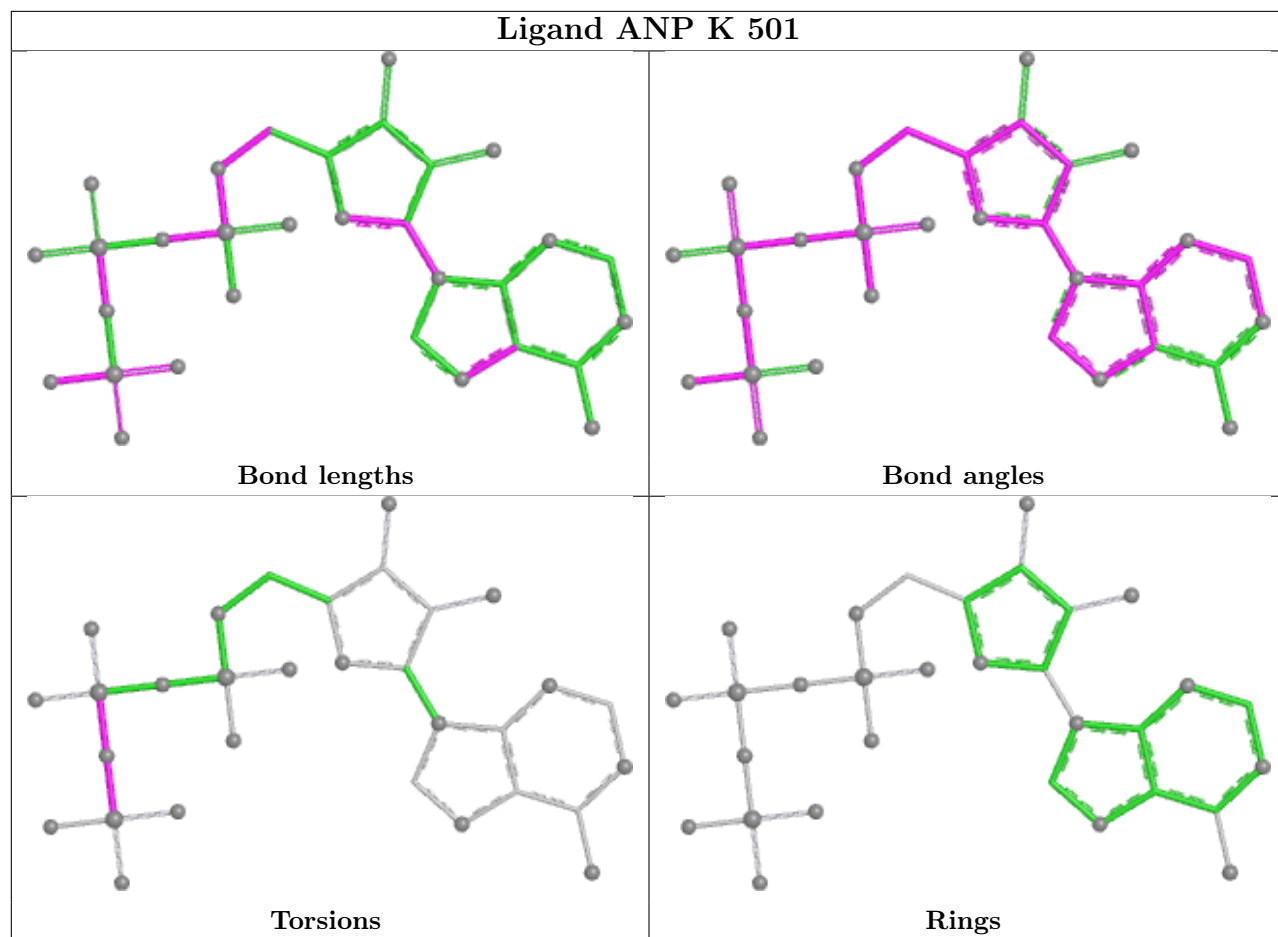


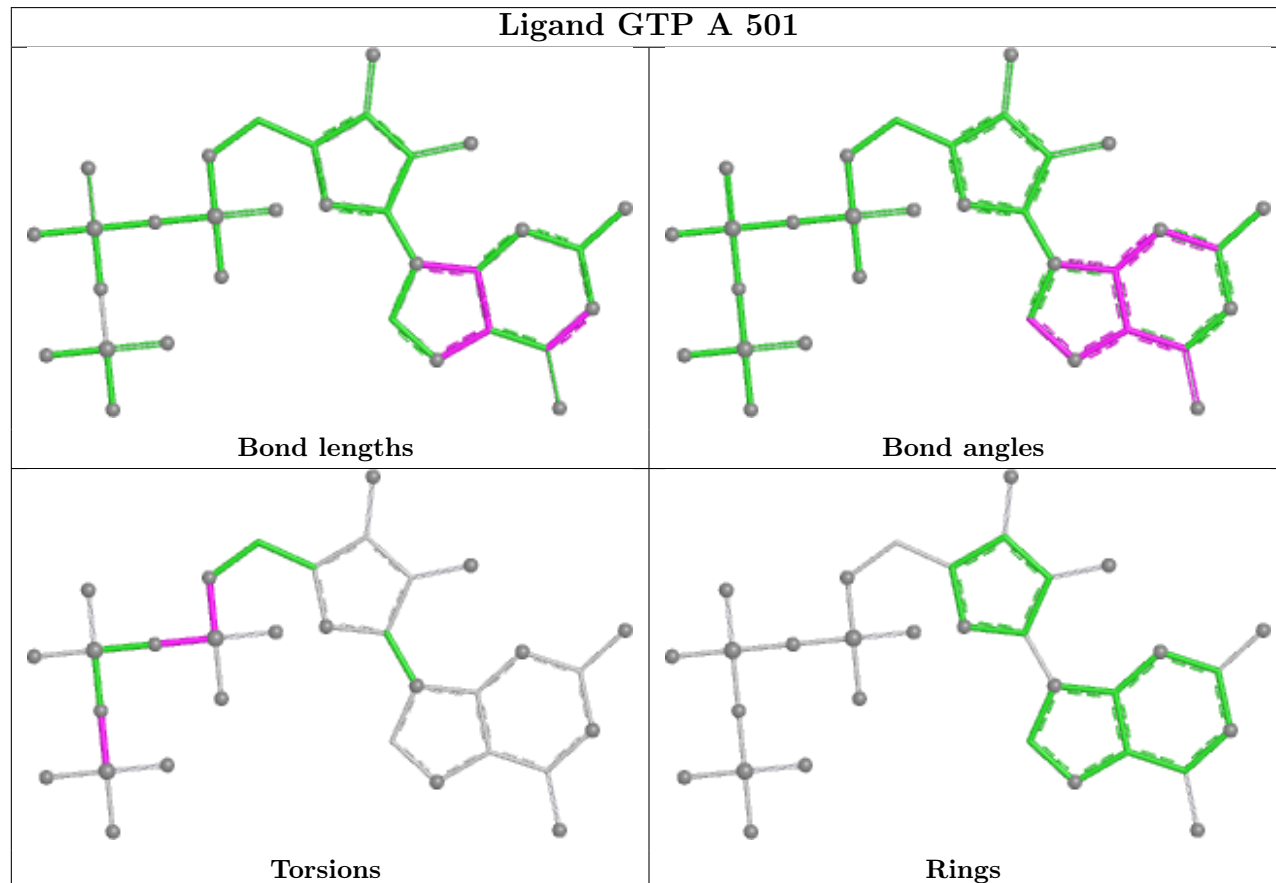
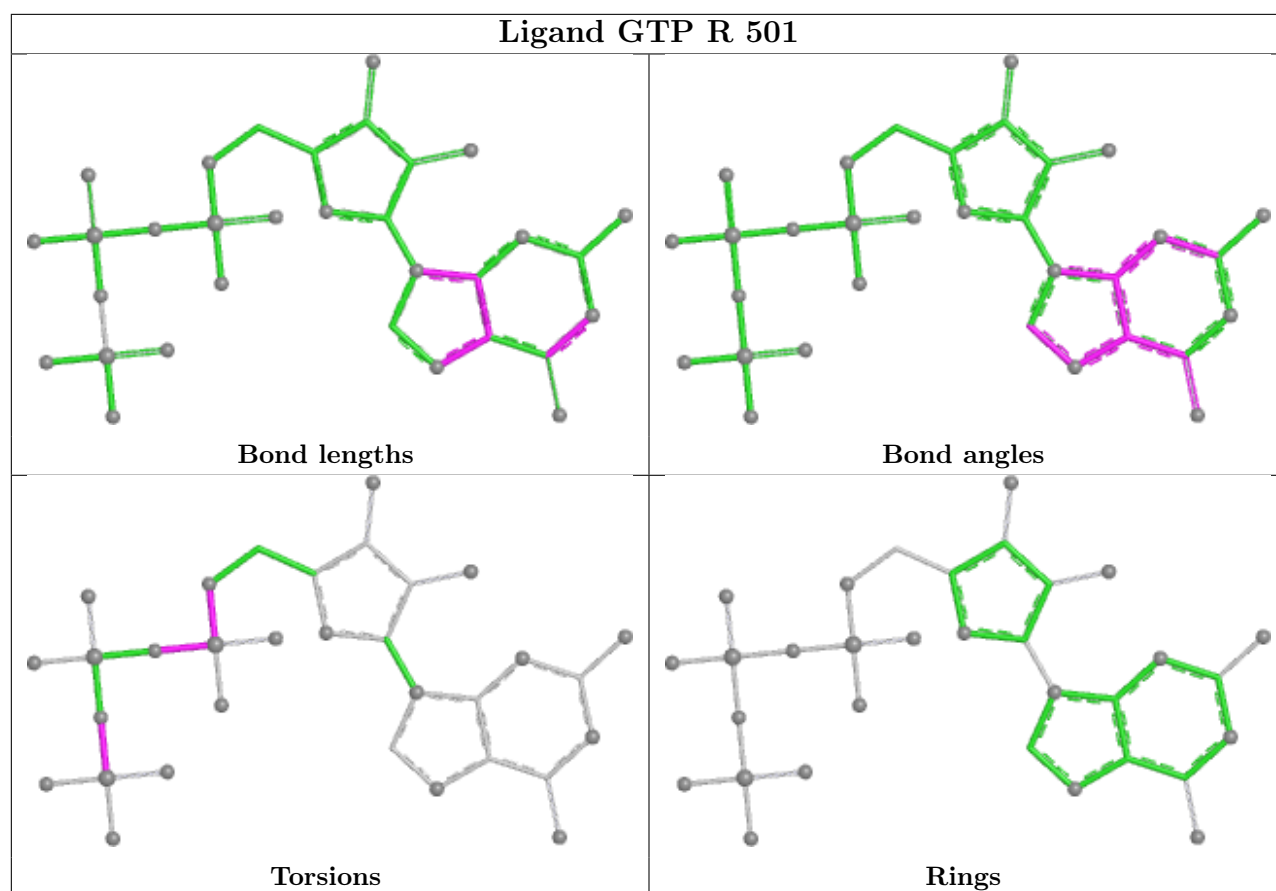




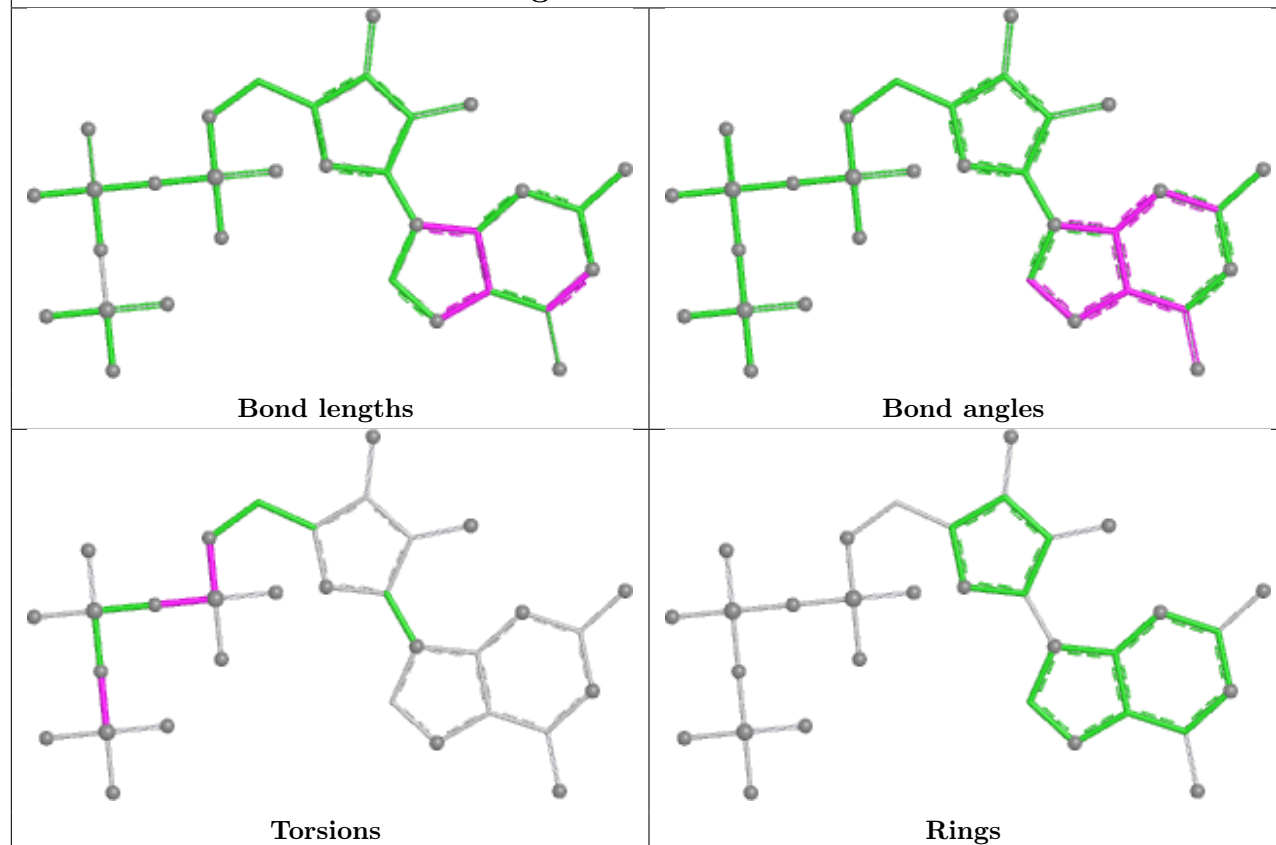




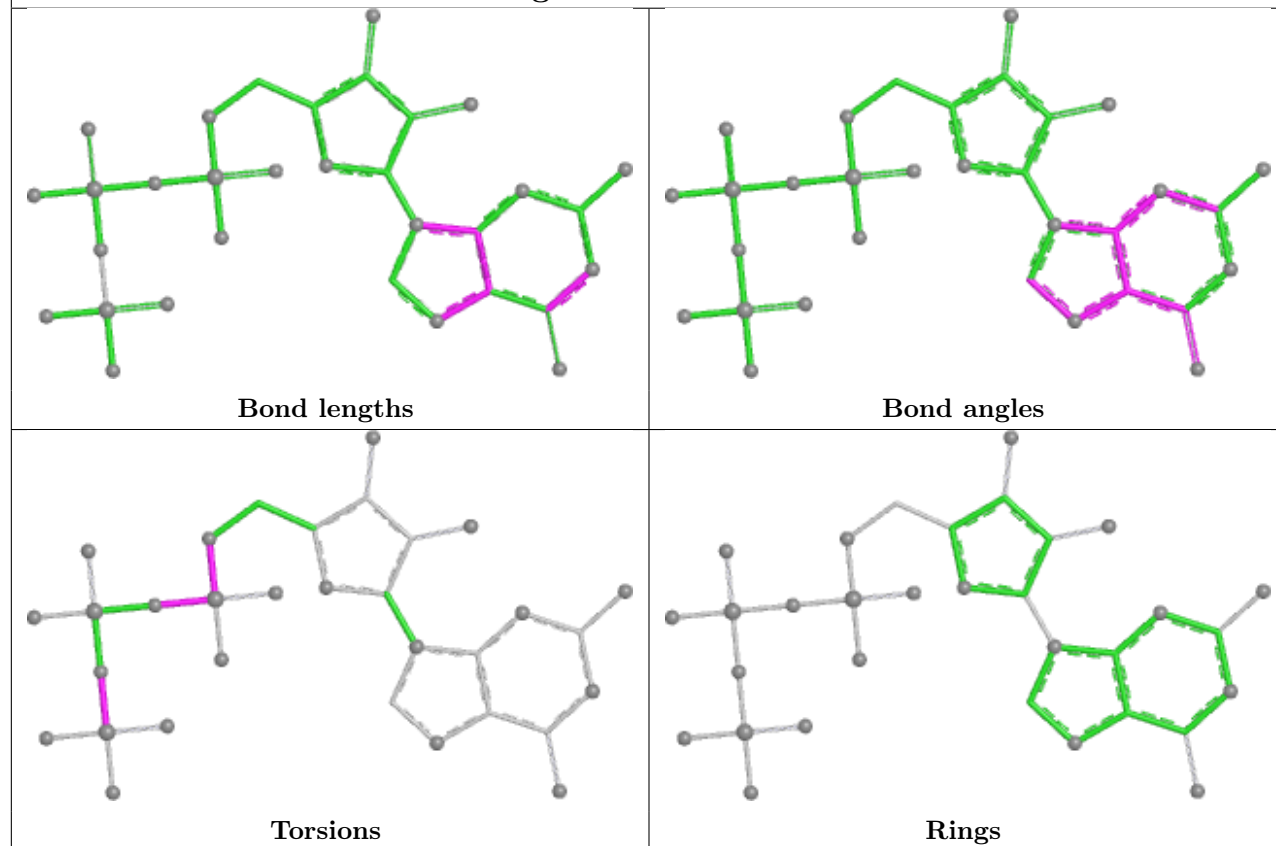


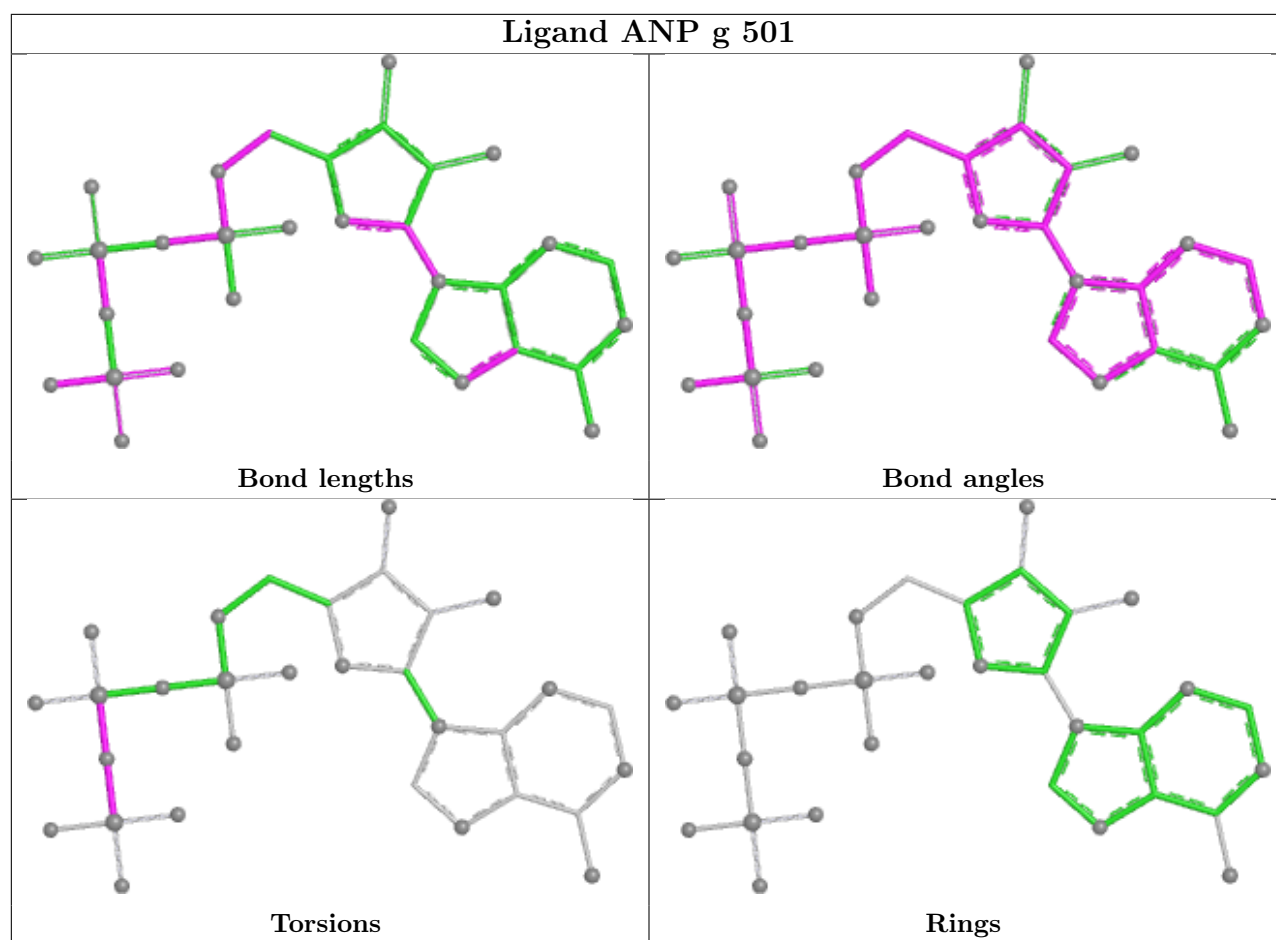


Ligand GTP P 501



Ligand GTP E 501





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.

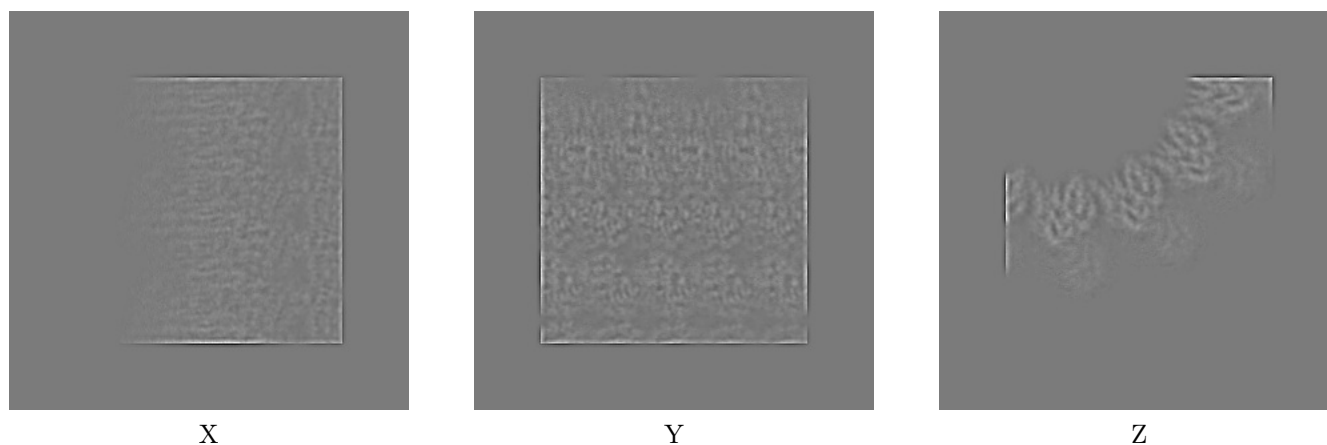
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24667. 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](#)

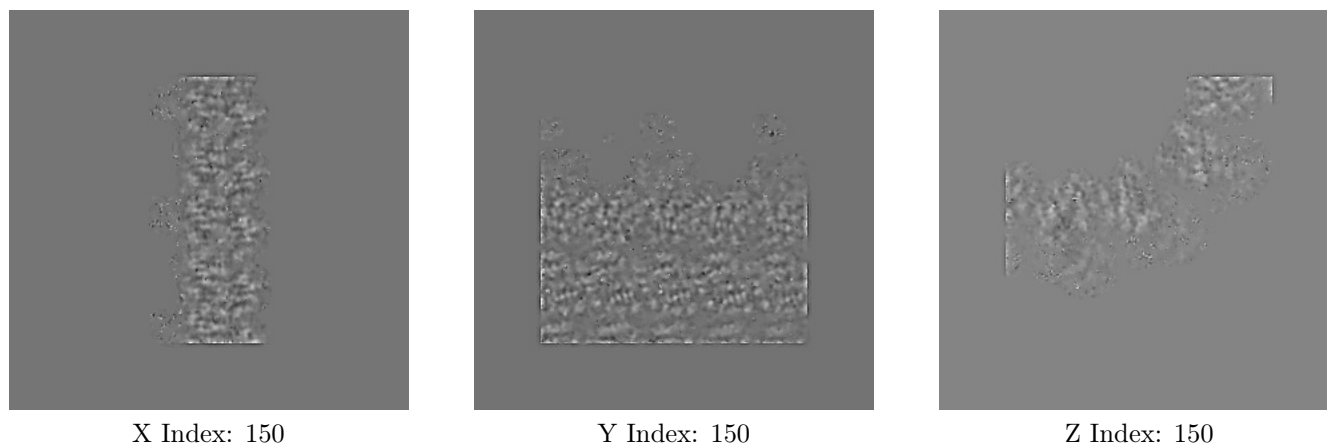
6.1.1 Primary map



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

6.2 Central slices [i](#)

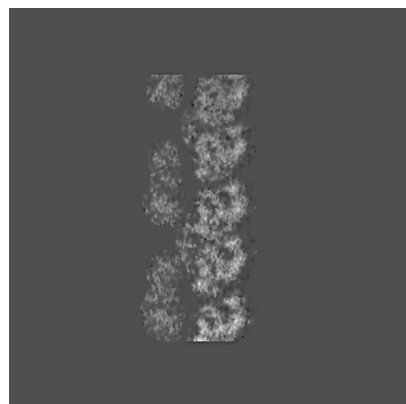
6.2.1 Primary map



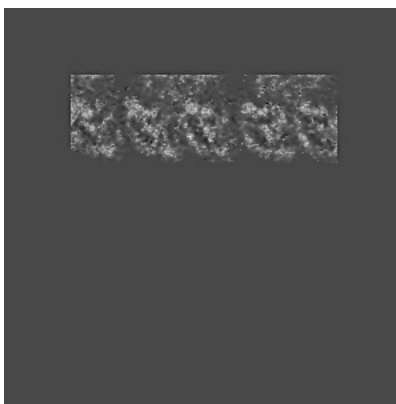
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

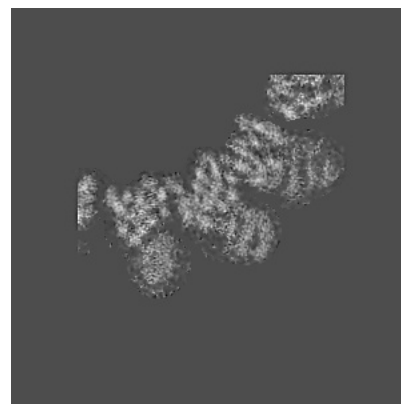
6.3.1 Primary map



X Index: 50



Y Index: 249

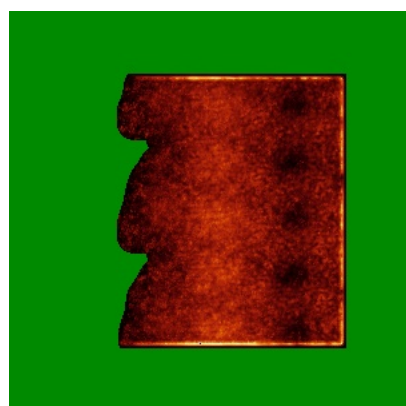


Z Index: 50

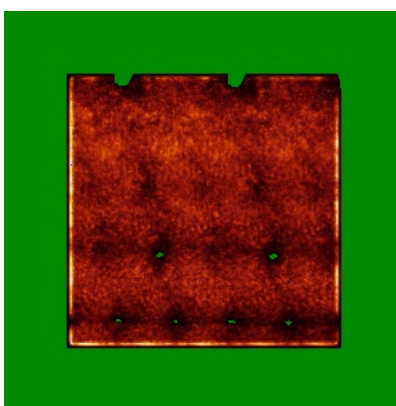
The images above show the largest variance slices of the map in three orthogonal directions.

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

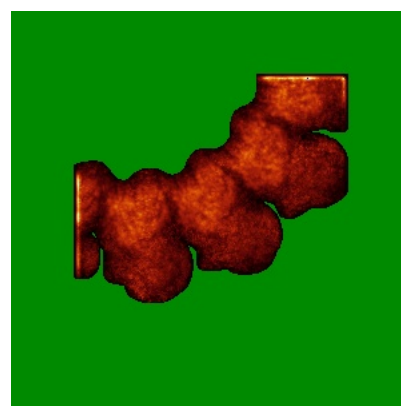
6.4.1 Primary map



X



Y

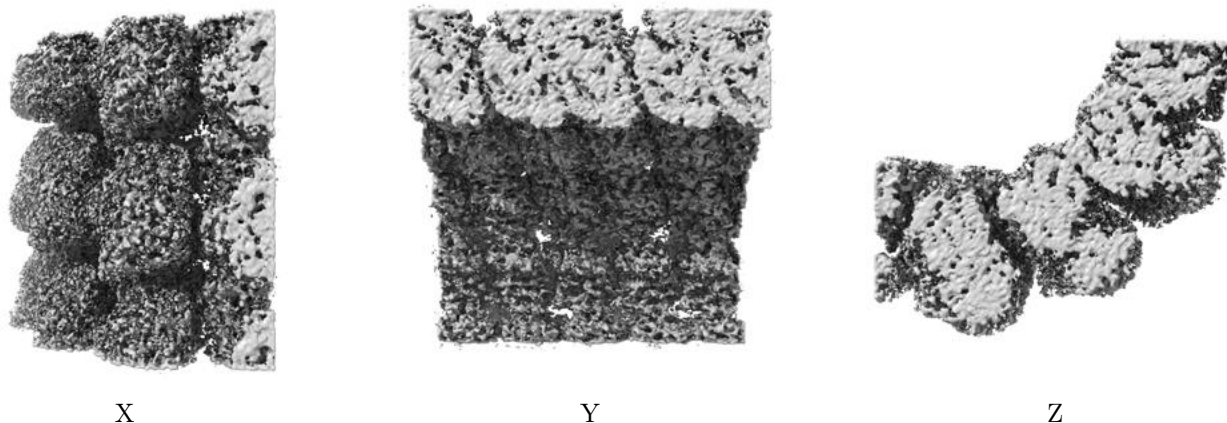


Z

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

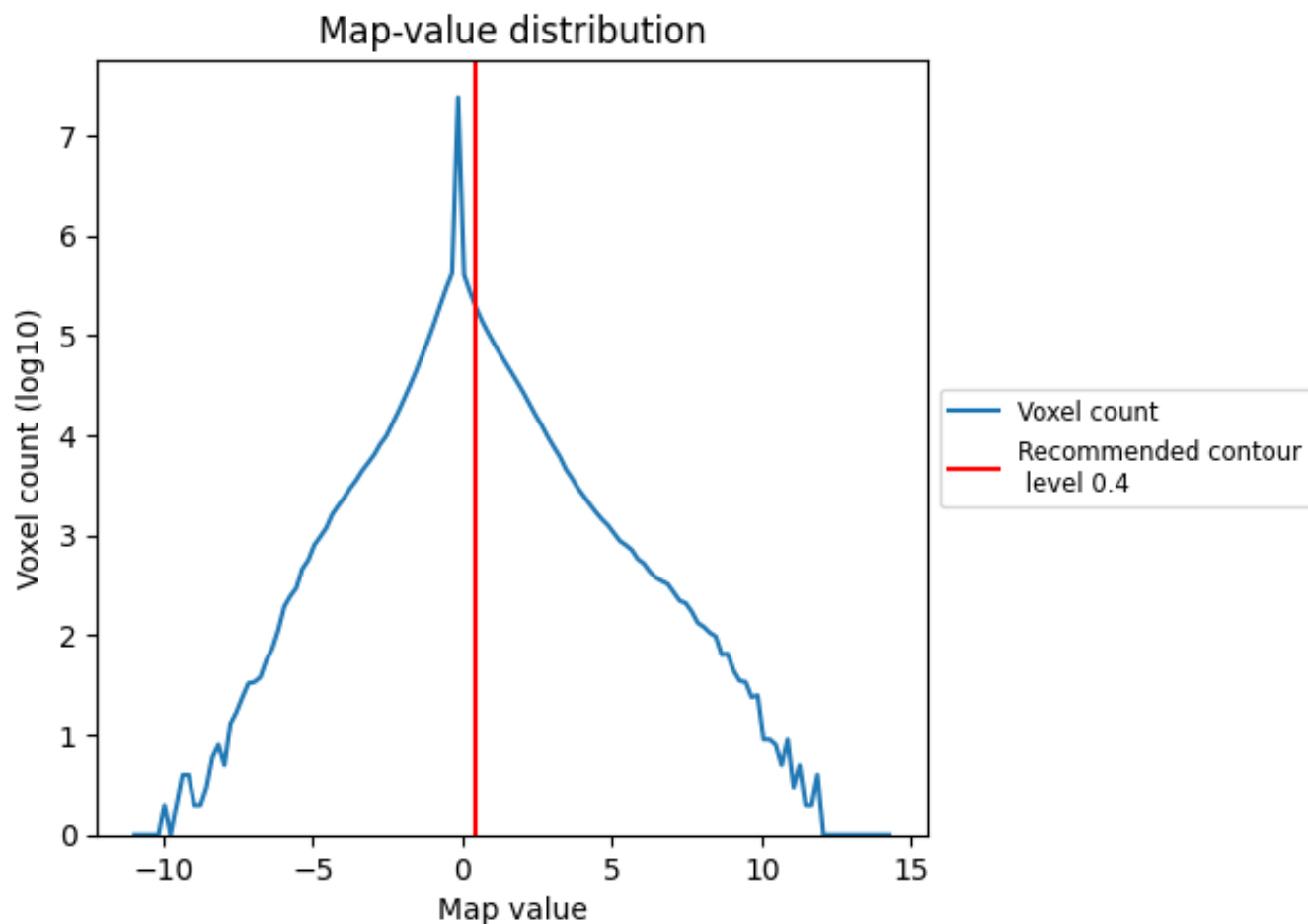
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

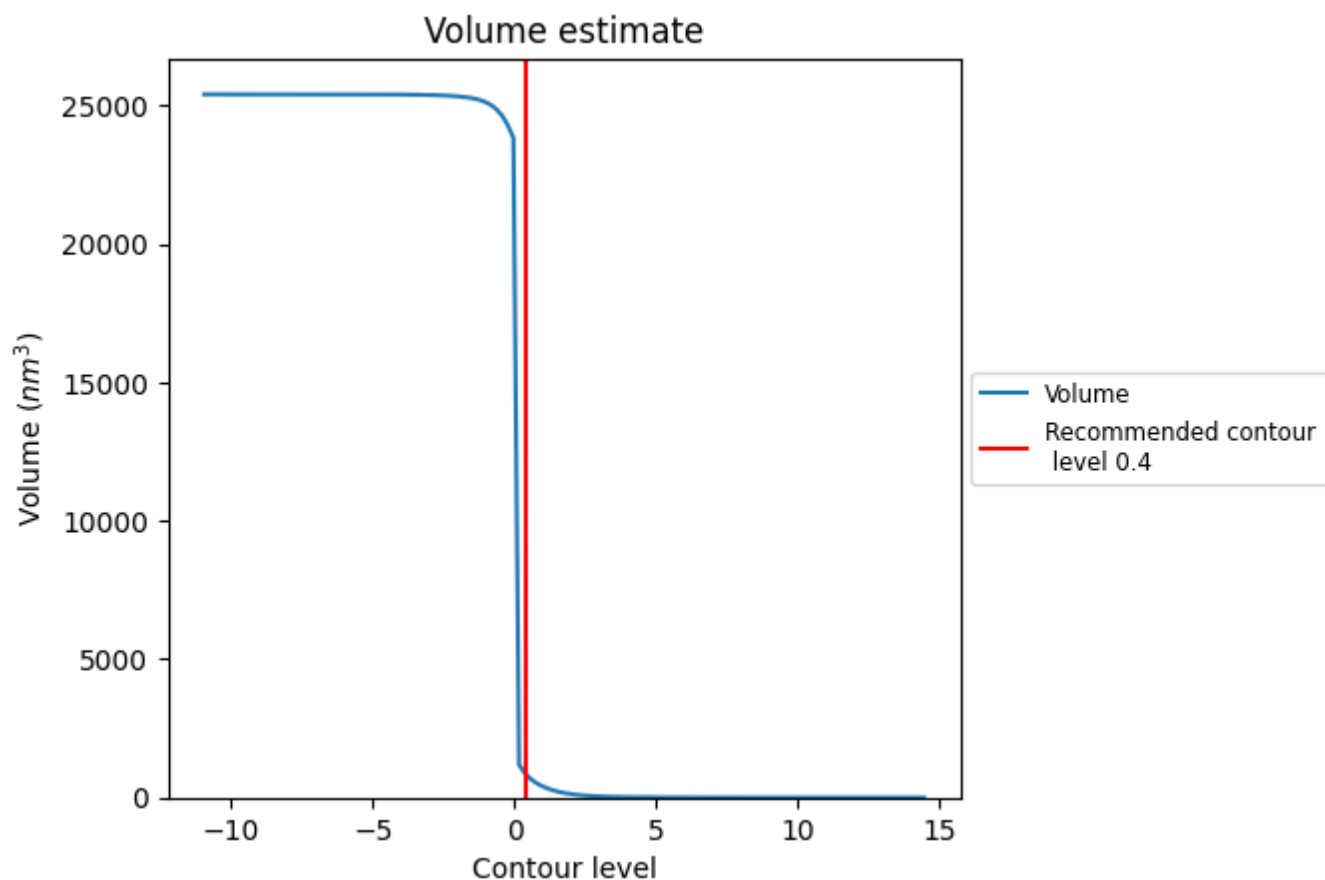
This section contains the results of statistical analysis of the map.

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.

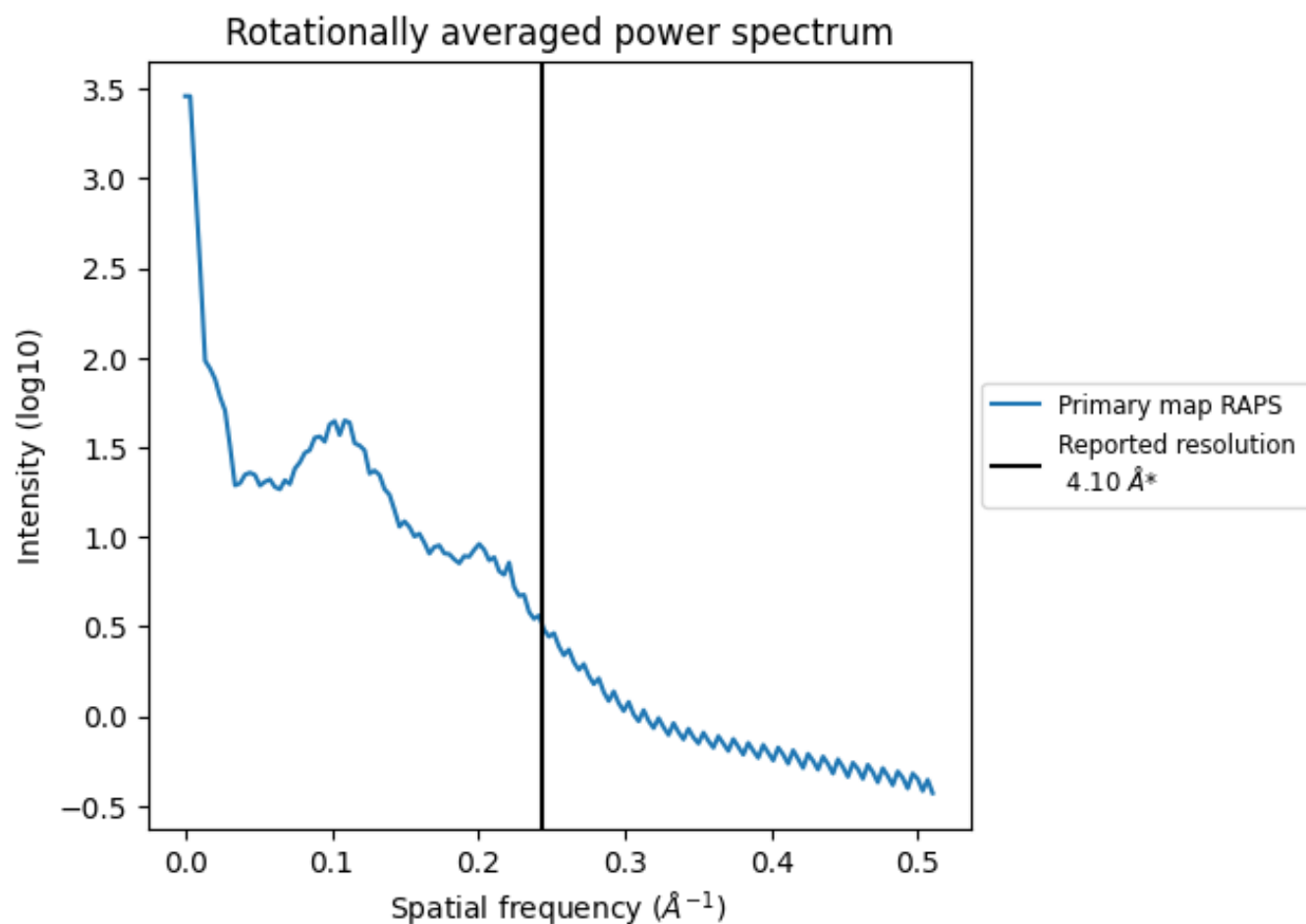
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 857 nm³; this corresponds to an approximate mass of 774 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 0.244 Å⁻¹

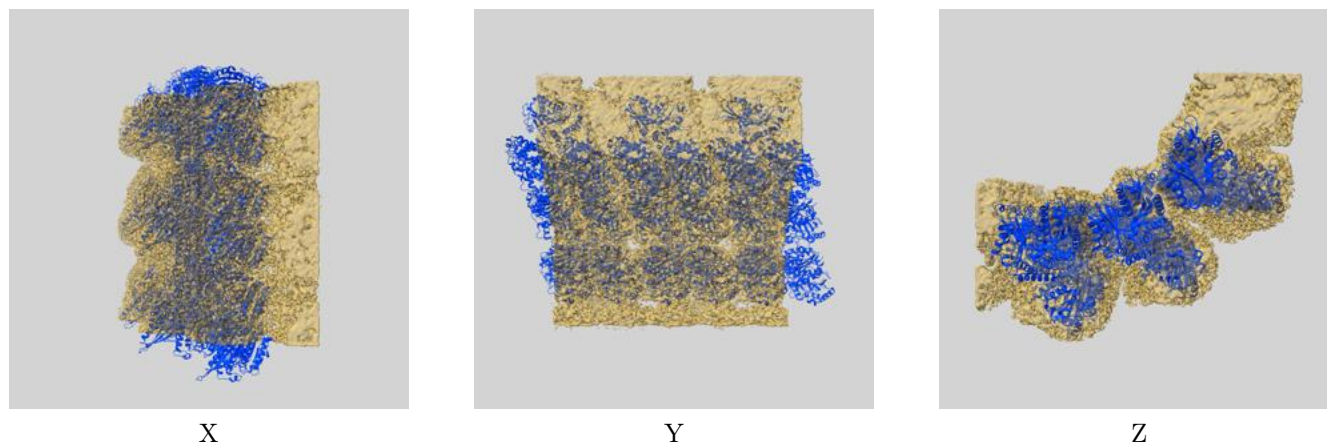
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

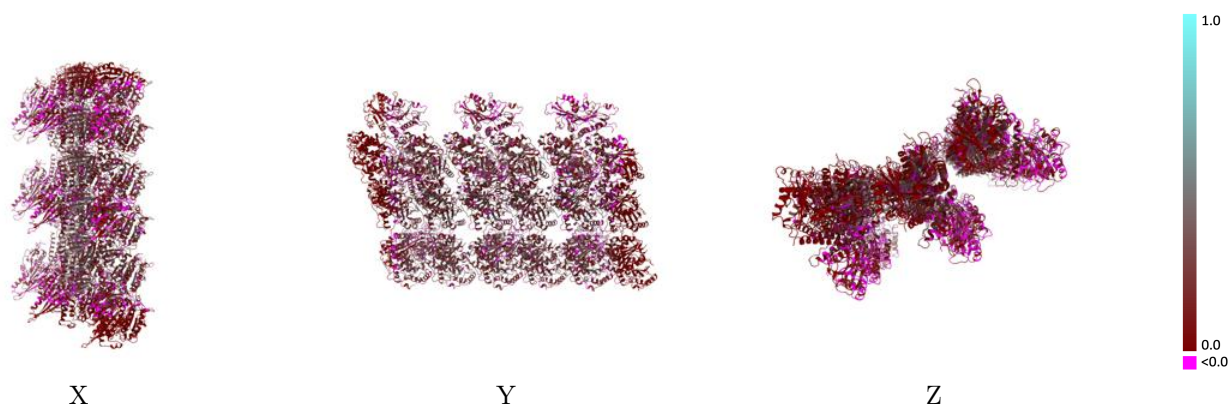
This section contains information regarding the fit between EMDB map EMD-24667 and PDB model 7RS6. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



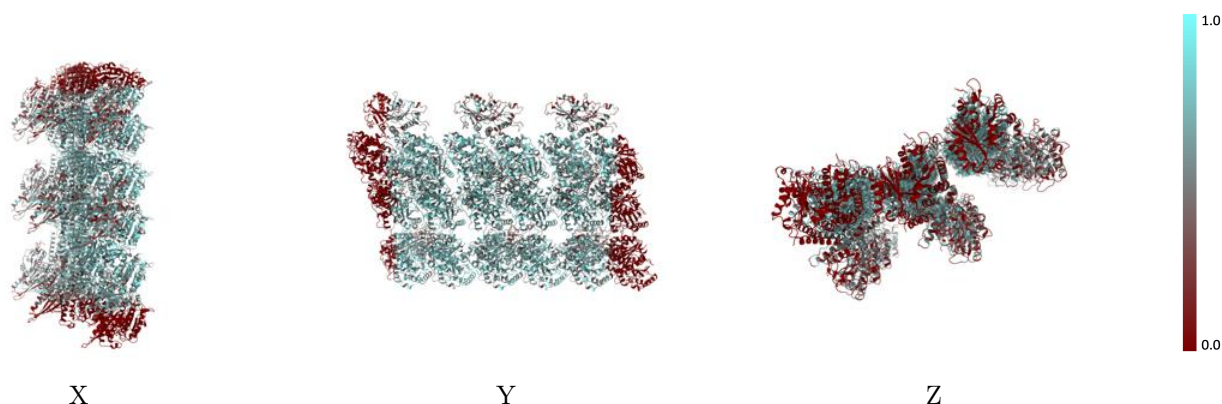
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



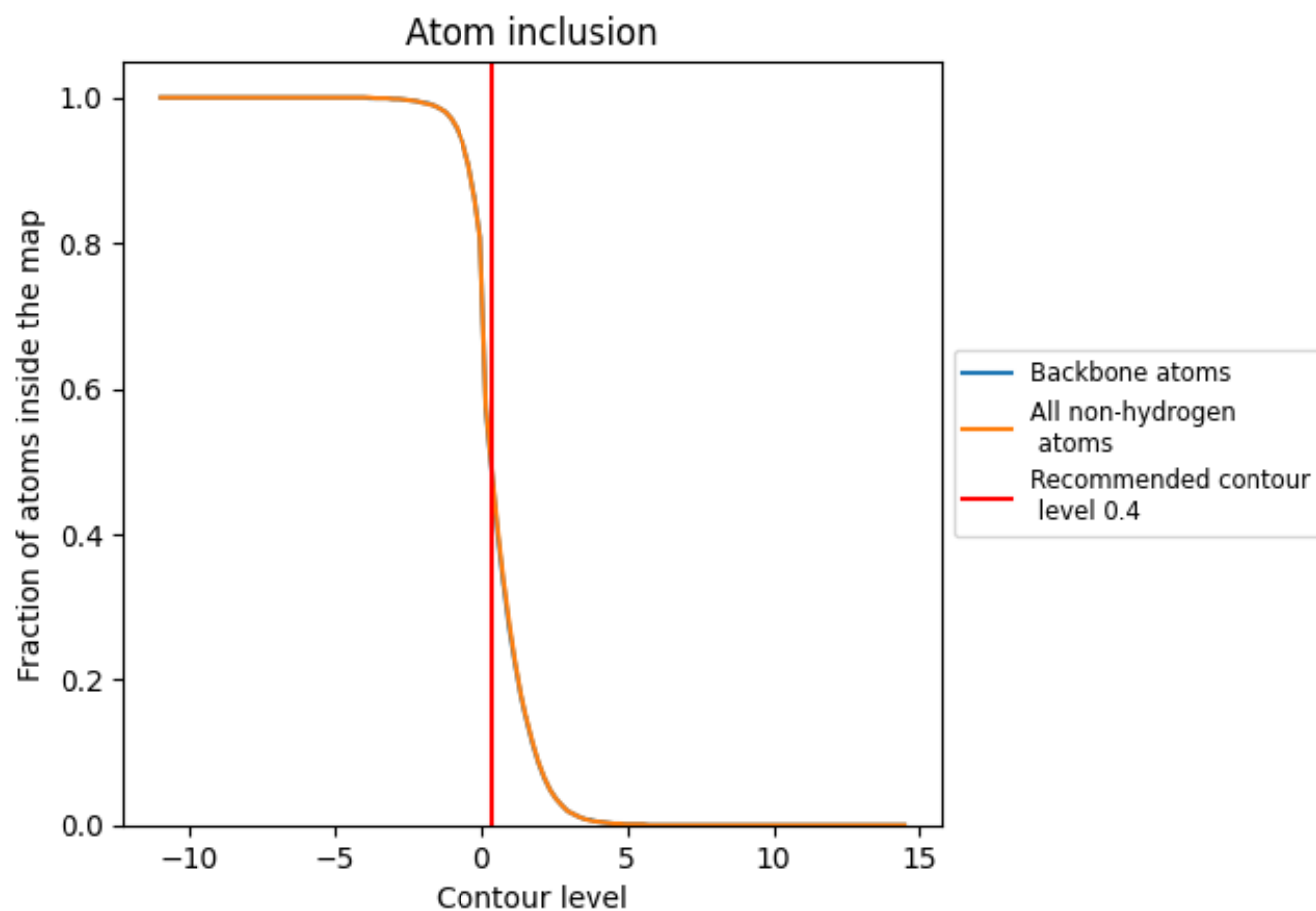
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 47% of all backbone atoms, 48% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4780	 0.1410
A	 0.6600	 0.2170
B	 0.6650	 0.2200
C	 0.6580	 0.2050
D	 0.6620	 0.2070
E	 0.6590	 0.2190
F	 0.6650	 0.2210
G	 0.6770	 0.2270
H	 0.3240	 0.0950
I	 0.1670	 0.0490
J	 0.6510	 0.2040
K	 0.4100	 0.0780
L	 0.6730	 0.2290
M	 0.1560	 0.0530
N	 0.3190	 0.0960
O	 0.6480	 0.2020
P	 0.6740	 0.2250
Q	 0.4800	 0.1530
R	 0.0530	 0.0190
S	 0.6390	 0.1880
a	 0.4290	 0.0820
b	 0.4120	 0.0750
c	 0.3400	 0.0610
d	 0.3580	 0.0670
e	 0.2530	 0.0560
f	 0.3840	 0.0740
g	 0.4250	 0.0890
h	 0.3260	 0.0560

