



# wwPDB X-ray Structure Validation Summary Report

Mar 5, 2026 – 09:03 PM UTC

PDB ID : 7TEN / pdb\_00007ten  
Title : Crystal structure of the *Listeria monocytogenes* GS-Met-Sox-P- ADP complex to 3.5 Angstrom  
Authors : Schumacher, M.A.  
Deposited on : 2022-01-05  
Resolution : 3.50 Å (reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

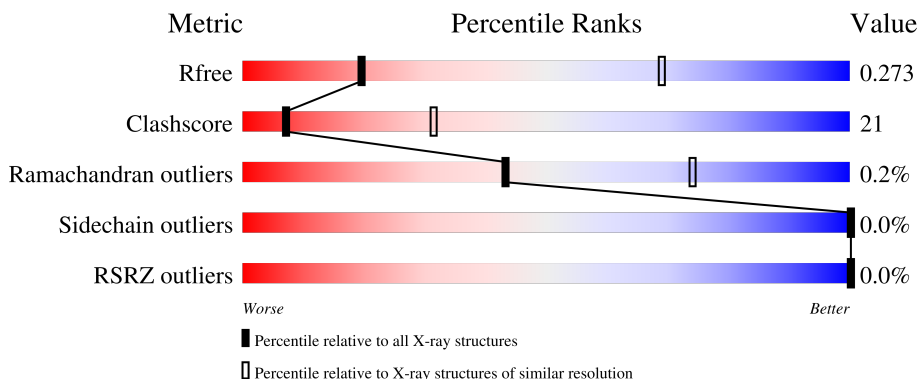
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


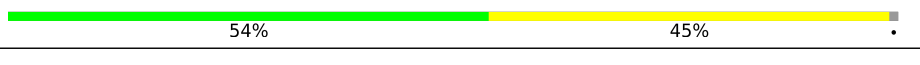

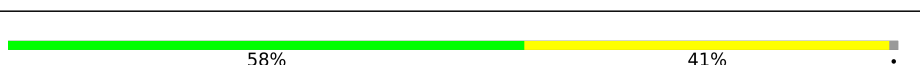

The reported resolution of this entry is 3.50 Å.

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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	447	
1	B	447	
1	D	447	
1	E	447	
1	H	447	

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Mol	Chain	Length	Quality of chain	
1	J	447		.
1	M	447		.
1	O	447		.
1	Q	447		.
1	S	447		.
1	U	447		.
1	W	447		.

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 42583 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Glutamine synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	442	3512	2248	586	660	18	0	0	0
1	E	442	3496	2243	585	650	18	0	0	0
1	B	442	3505	2246	580	661	18	0	0	0
1	D	442	3509	2248	587	656	18	0	0	0
1	H	442	3525	2257	584	666	18	0	0	0
1	J	442	3496	2241	587	650	18	0	0	0
1	M	442	3501	2241	583	659	18	0	0	0
1	O	442	3508	2247	588	655	18	0	0	0
1	Q	442	3503	2243	581	661	18	0	0	0
1	S	442	3497	2242	588	649	18	0	0	0
1	U	442	3515	2250	586	661	18	0	0	0
1	W	442	3512	2249	587	658	18	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A0A5D5GA79
A	-1	SER	-	expression tag	UNP A0A5D5GA79
A	0	HIS	-	expression tag	UNP A0A5D5GA79
A	402	ASN	ASP	conflict	UNP A0A5D5GA79
E	-2	GLY	-	expression tag	UNP A0A5D5GA79

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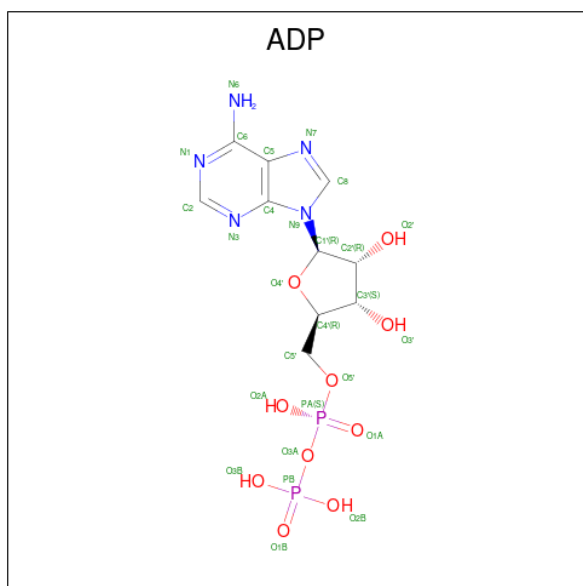
Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	SER	-	expression tag	UNP A0A5D5GA79
E	0	HIS	-	expression tag	UNP A0A5D5GA79
E	402	ASN	ASP	conflict	UNP A0A5D5GA79
B	-2	GLY	-	expression tag	UNP A0A5D5GA79
B	-1	SER	-	expression tag	UNP A0A5D5GA79
B	0	HIS	-	expression tag	UNP A0A5D5GA79
B	402	ASN	ASP	conflict	UNP A0A5D5GA79
D	-2	GLY	-	expression tag	UNP A0A5D5GA79
D	-1	SER	-	expression tag	UNP A0A5D5GA79
D	0	HIS	-	expression tag	UNP A0A5D5GA79
D	402	ASN	ASP	conflict	UNP A0A5D5GA79
H	-2	GLY	-	expression tag	UNP A0A5D5GA79
H	-1	SER	-	expression tag	UNP A0A5D5GA79
H	0	HIS	-	expression tag	UNP A0A5D5GA79
H	402	ASN	ASP	conflict	UNP A0A5D5GA79
J	-2	GLY	-	expression tag	UNP A0A5D5GA79
J	-1	SER	-	expression tag	UNP A0A5D5GA79
J	0	HIS	-	expression tag	UNP A0A5D5GA79
J	402	ASN	ASP	conflict	UNP A0A5D5GA79
M	-2	GLY	-	expression tag	UNP A0A5D5GA79
M	-1	SER	-	expression tag	UNP A0A5D5GA79
M	0	HIS	-	expression tag	UNP A0A5D5GA79
M	402	ASN	ASP	conflict	UNP A0A5D5GA79
O	-2	GLY	-	expression tag	UNP A0A5D5GA79
O	-1	SER	-	expression tag	UNP A0A5D5GA79
O	0	HIS	-	expression tag	UNP A0A5D5GA79
O	402	ASN	ASP	conflict	UNP A0A5D5GA79
Q	-2	GLY	-	expression tag	UNP A0A5D5GA79
Q	-1	SER	-	expression tag	UNP A0A5D5GA79
Q	0	HIS	-	expression tag	UNP A0A5D5GA79
Q	402	ASN	ASP	conflict	UNP A0A5D5GA79
S	-2	GLY	-	expression tag	UNP A0A5D5GA79
S	-1	SER	-	expression tag	UNP A0A5D5GA79
S	0	HIS	-	expression tag	UNP A0A5D5GA79
S	402	ASN	ASP	conflict	UNP A0A5D5GA79
U	-2	GLY	-	expression tag	UNP A0A5D5GA79
U	-1	SER	-	expression tag	UNP A0A5D5GA79
U	0	HIS	-	expression tag	UNP A0A5D5GA79
U	402	ASN	ASP	conflict	UNP A0A5D5GA79
W	-2	GLY	-	expression tag	UNP A0A5D5GA79
W	-1	SER	-	expression tag	UNP A0A5D5GA79
W	0	HIS	-	expression tag	UNP A0A5D5GA79

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Chain	Residue	Modelled	Actual	Comment	Reference
W	402	ASN	ASP	conflict	UNP A0A5D5GA79

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



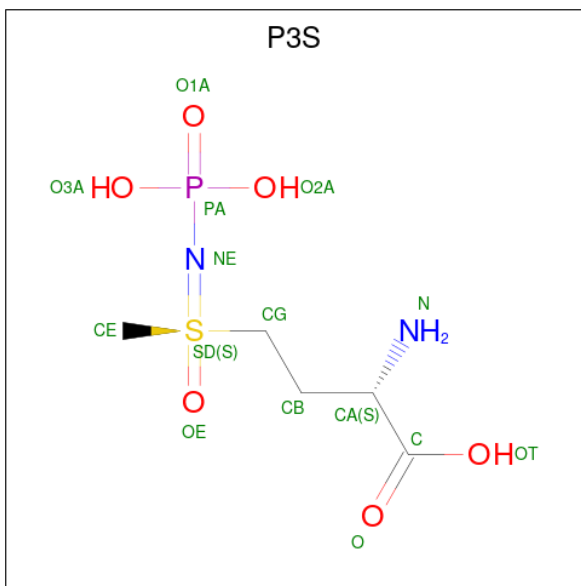
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	J	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	M	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	O	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	Q	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	S	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	U	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	W	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is L-METHIONINE-S-SULFOXIMINE PHOSPHATE (CCD ID: P3S) (formula:  $C_5H_{13}N_2O_6PS$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
3	A	1	Total	C	N	O	P	S	0	0
			15	5	2	6	1	1		
3	E	1	Total	C	N	O	P	S	0	0
			15	5	2	6	1	1		
3	B	1	Total	C	N	O	P	S	0	0
			15	5	2	6	1	1		
3	D	1	Total	C	N	O	P	S	0	0
			15	5	2	6	1	1		
3	H	1	Total	C	N	O	P	S	0	0
			15	5	2	6	1	1		
3	J	1	Total	C	N	O	P	S	0	0
			15	5	2	6	1	1		
3	M	1	Total	C	N	O	P	S	0	0
			15	5	2	6	1	1		
3	O	1	Total	C	N	O	P	S	0	0
			15	5	2	6	1	1		
3	Q	1	Total	C	N	O	P	S	0	0
			15	5	2	6	1	1		

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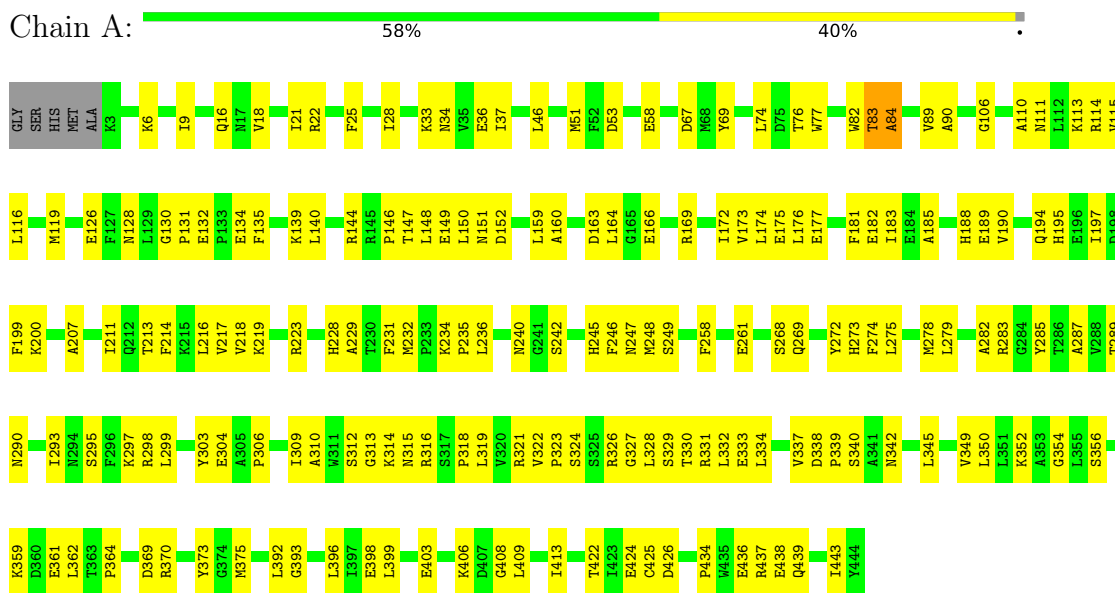
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
3	S	1	Total 15	5	2	6	1	1	0	0
3	U	1	Total 15	5	2	6	1	1	0	0
3	W	1	Total 15	5	2	6	1	1	0	0

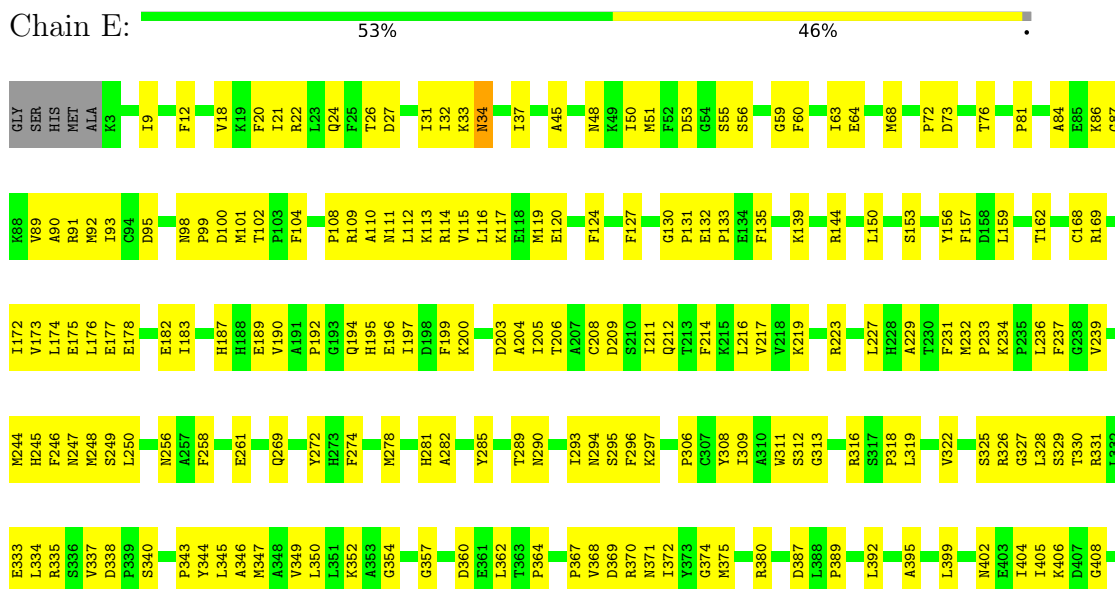
### 3 Residue-property plots [\(i\)](#)

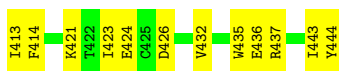
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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: Glutamine synthetase



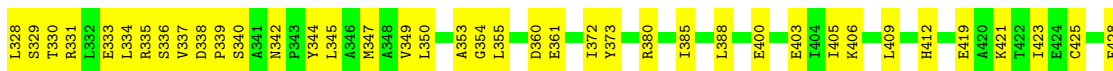
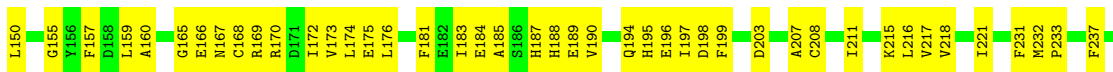
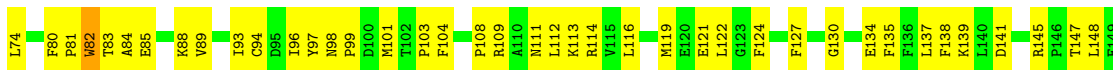
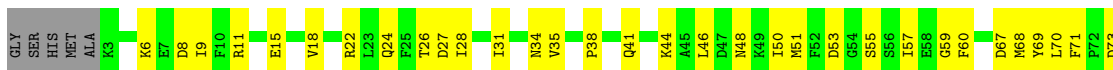
- Molecule 1: Glutamine synthetase





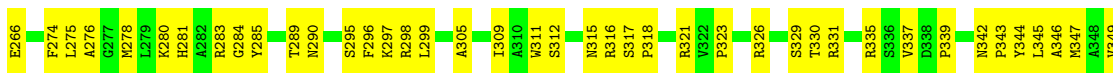
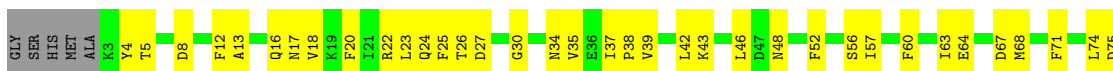
- Molecule 1: Glutamine synthetase

Chain B: 54% 45%



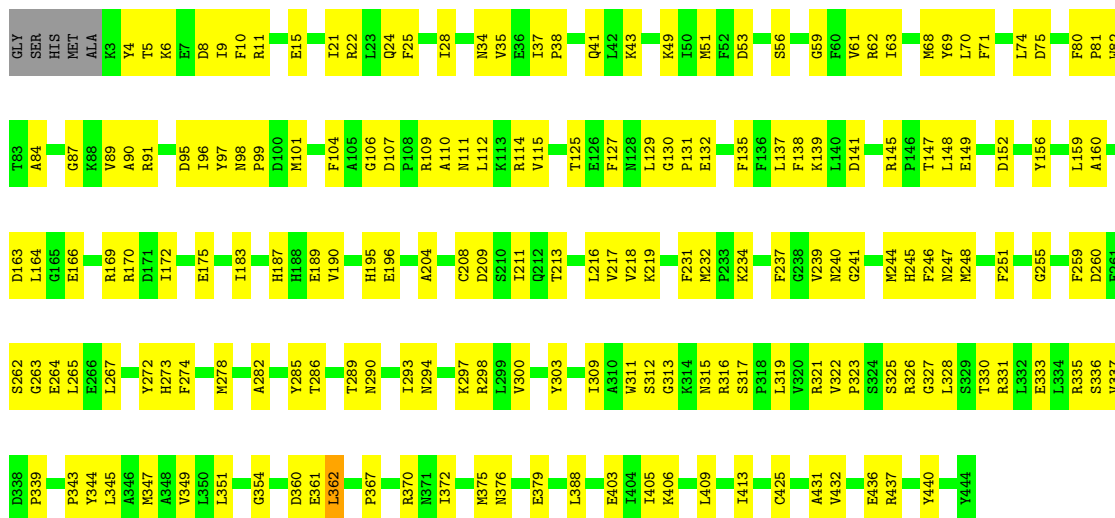
- Molecule 1: Glutamine synthetase

Chain D: 57% 42%



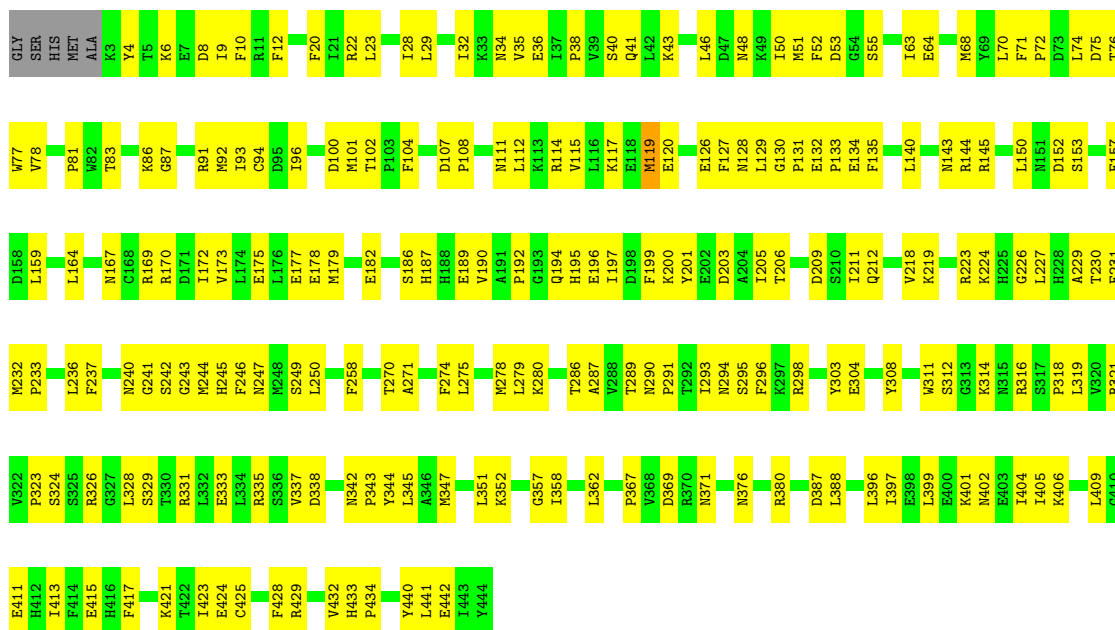
- Molecule 1: Glutamine synthetase

Chain H: 58% 41%



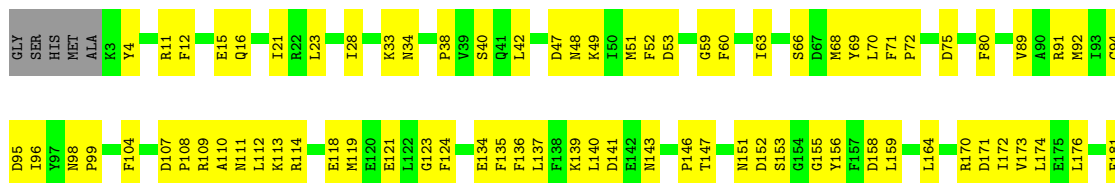
- Molecule 1: Glutamine synthetase

Chain J: 52% 47%



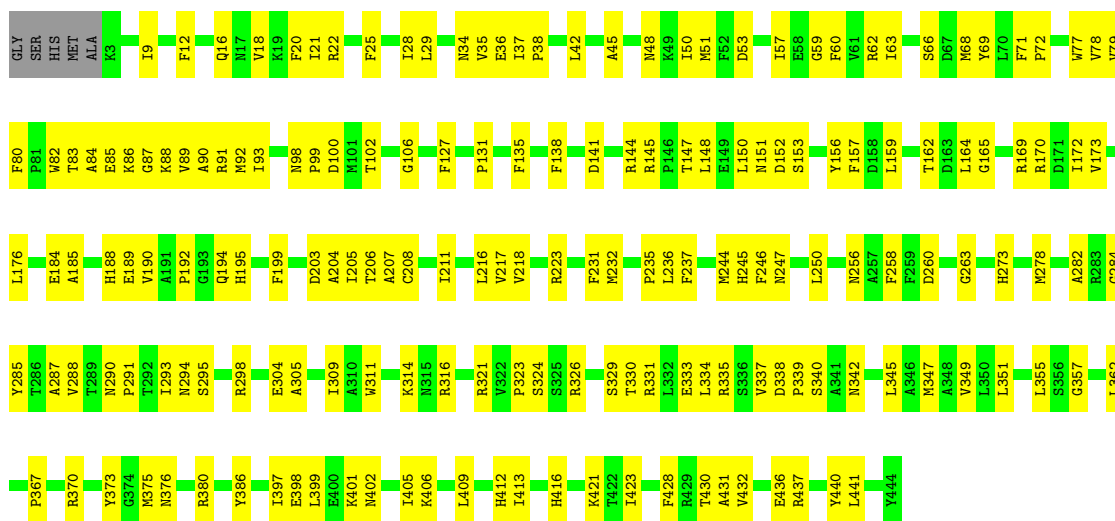
- Molecule 1: Glutamine synthetase

Chain M: 54% 45%

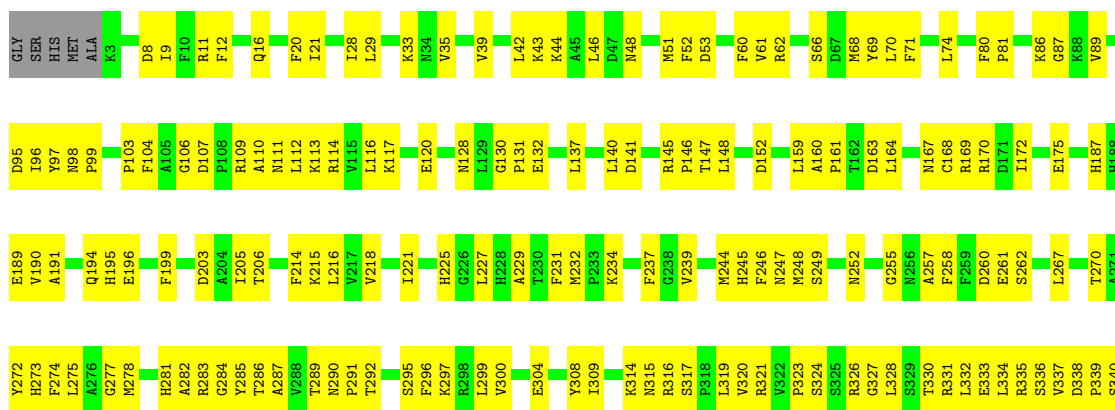




• Molecule 1: Glutamine synthetase

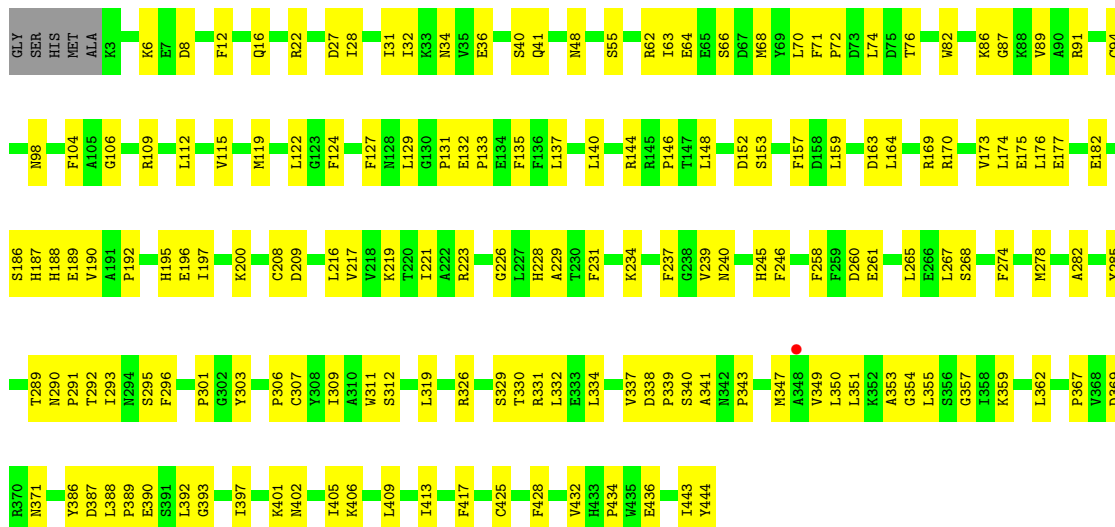


• Molecule 1: Glutamine synthetase

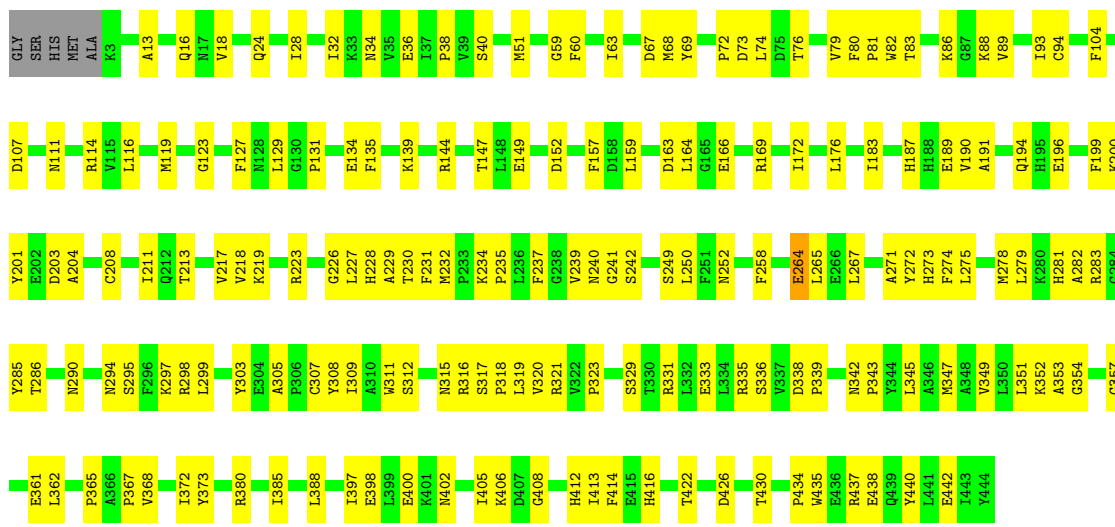




• Molecule 1: Glutamine synthetase



• Molecule 1: Glutamine synthetase



• Molecule 1: Glutamine synthetase



R91	M92	I93	C94	D95	I96	Y97	M98	P99	D100	M101	T102	F103	F104	D107	R114	V115	L116	K117	E118	M119	E120	T125	E126	F127	N128	L129	G130	P131	E132	P133	E134	F135	F136	L137	L140	L146	T147	L148	S153	G154	G155	L159	L164	G165	E166	M167	C168	R169	I172	V173
L174	E175	L176	M179	E182	I183	H187	H188	E189	V190	A191	P192	G193	Q194	H195	E196	K200	A207	C208	D209	S210	I211	V218	H228	F231	G238	V239	M240	G243	M244	N247	M248	S249	L250	F251	G255	F258	F259	D260	E261	L267	Y272	H273	F274	L275						
M278	H281	A282	R283	G284	Y285	T286	A287	V288	T289	Y290	P291	T292	S295	F296	Y303	W311	S317	P318	L319	V320	R321	R326	S329	T330	R331	V337	D338	P339	S340	A341	N342	P343	Y344	A348	V349	L350	L351	K352	A353	G354	L355	P367	M375	M376	E379	R380				
I385	Y386	D387	L388	P389	L392	L399	I405	K406	D407	G408	L409	K421	T422	C425	D426	T430	A431	V432	H433	P434	W435	E436	R437	E438	L441	E442	I443	Y444																						

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	112.61Å 137.61Å 138.02Å 60.75° 87.16° 68.40°	Depositor
Resolution (Å)	63.88 – 3.50 63.88 – 3.50	Depositor EDS
% Data completeness (in resolution range)	74.3 (63.88-3.50) 74.3 (63.88-3.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.18	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 3.49Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.201 , 0.273 0.202 , 0.273	Depositor DCC
$R_{free}$ test set	1990 reflections (2.38%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	98.8	Xtrriage
Anisotropy	0.087	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 68.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	42583	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	113.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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: P3S, ADP

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	0.22	0/3597	0.51	0/4867
1	B	0.22	0/3590	0.54	0/4859
1	D	0.21	0/3595	0.49	0/4864
1	E	0.28	1/3583 (0.0%)	0.54	0/4851
1	H	0.26	0/3610	0.56	0/4883
1	J	0.22	0/3582	0.52	0/4848
1	M	0.21	0/3585	0.51	0/4852
1	O	0.22	0/3594	0.51	0/4863
1	Q	0.21	0/3587	0.51	0/4854
1	S	0.22	0/3583	0.49	0/4849
1	U	0.22	0/3600	0.49	0/4870
1	W	0.22	0/3598	0.50	0/4868
All	All	0.23	1/43104 (0.0%)	0.52	0/58328

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	E	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	364	PRO	CA-C	7.44	1.59	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	83	THR	Peptide
1	E	34	ASN	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3512	0	3421	153	0
1	B	3505	0	3399	178	0
1	D	3509	0	3417	156	0
1	E	3496	0	3395	180	0
1	H	3525	0	3433	153	0
1	J	3496	0	3404	186	0
1	M	3501	0	3399	177	0
1	O	3508	0	3418	159	0
1	Q	3503	0	3402	149	0
1	S	3497	0	3407	130	0
1	U	3515	0	3420	158	0
1	W	3512	0	3419	143	0
2	A	27	0	12	5	0
2	B	27	0	12	5	0
2	D	27	0	12	2	0
2	E	27	0	12	2	0
2	H	27	0	12	3	0
2	J	27	0	12	5	0
2	M	27	0	12	3	0
2	O	27	0	12	4	0
2	Q	27	0	12	1	0
2	S	27	0	12	2	0
2	U	27	0	12	1	0
2	W	27	0	12	0	0
3	A	15	0	10	1	0
3	B	15	0	10	4	0
3	D	15	0	10	2	0
3	E	15	0	8	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	15	0	10	2	0
3	J	15	0	10	1	0
3	M	15	0	10	5	0
3	O	15	0	10	3	0
3	Q	15	0	10	1	0
3	S	15	0	10	1	0
3	U	15	0	10	5	0
3	W	15	0	10	0	0
All	All	42583	0	41196	1741	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 21.

The worst 5 of 1741 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:51:MET:HE3	1:U:69:TYR:CZ	1.70	1.25
1:M:170:ARG:NH1	1:O:36:GLU:OE2	1.97	0.98
1:U:51:MET:CE	1:U:69:TYR:CZ	2.49	0.96
1:U:51:MET:CE	1:U:69:TYR:CE1	2.50	0.95
1:D:119:MET:HG2	1:D:351:LEU:HD21	1.49	0.95

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	440/447 (98%)	389 (88%)	49 (11%)	2 (0%)	24	57
1	B	440/447 (98%)	393 (89%)	46 (10%)	1 (0%)	43	74
1	D	440/447 (98%)	397 (90%)	43 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	440/447 (98%)	396 (90%)	44 (10%)	0	100	100
1	H	440/447 (98%)	393 (89%)	45 (10%)	2 (0%)	24	57
1	J	440/447 (98%)	393 (89%)	47 (11%)	0	100	100
1	M	440/447 (98%)	390 (89%)	48 (11%)	2 (0%)	24	57
1	O	440/447 (98%)	404 (92%)	36 (8%)	0	100	100
1	Q	440/447 (98%)	390 (89%)	50 (11%)	0	100	100
1	S	440/447 (98%)	398 (90%)	42 (10%)	0	100	100
1	U	440/447 (98%)	388 (88%)	50 (11%)	2 (0%)	24	57
1	W	440/447 (98%)	412 (94%)	28 (6%)	0	100	100
All	All	5280/5364 (98%)	4743 (90%)	528 (10%)	9 (0%)	43	74

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	ALA
1	A	362	LEU
1	H	362	LEU
1	M	362	LEU
1	U	362	LEU

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	375/386 (97%)	375 (100%)	0	100	100
1	B	373/386 (97%)	373 (100%)	0	100	100
1	D	374/386 (97%)	374 (100%)	0	100	100
1	E	370/386 (96%)	370 (100%)	0	100	100
1	H	378/386 (98%)	378 (100%)	0	100	100
1	J	371/386 (96%)	370 (100%)	1 (0%)	86	83
1	M	372/386 (96%)	372 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	374/386 (97%)	374 (100%)	0	100	100
1	Q	373/386 (97%)	373 (100%)	0	100	100
1	S	371/386 (96%)	371 (100%)	0	100	100
1	U	375/386 (97%)	375 (100%)	0	100	100
1	W	375/386 (97%)	375 (100%)	0	100	100
All	All	4481/4632 (97%)	4480 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	119	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	41	GLN
1	Q	228	HIS
1	W	342	ASN
1	O	187	HIS
1	O	290	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](#)

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	ADP	S	501	-	28,29,29	1.43	4 (14%)	43,45,45	1.88	10 (23%)
3	P3S	J	502	-	11,14,14	1.94	3 (27%)	9,21,21	7.76	4 (44%)
3	P3S	M	502	-	11,14,14	1.84	3 (27%)	9,21,21	8.14	4 (44%)
2	ADP	A	501	-	28,29,29	1.42	4 (14%)	43,45,45	1.85	7 (16%)
3	P3S	A	502	-	11,14,14	2.05	3 (27%)	9,21,21	8.34	3 (33%)
3	P3S	H	502	-	11,14,14	1.85	2 (18%)	9,21,21	7.20	4 (44%)
2	ADP	H	501	-	28,29,29	1.39	4 (14%)	43,45,45	1.87	10 (23%)
3	P3S	B	502	-	11,14,14	1.91	2 (18%)	9,21,21	7.07	4 (44%)
2	ADP	M	501	-	28,29,29	1.39	4 (14%)	43,45,45	1.90	7 (16%)
2	ADP	W	501	-	28,29,29	1.44	4 (14%)	43,45,45	1.95	8 (18%)
3	P3S	W	502	-	11,14,14	1.97	3 (27%)	9,21,21	6.56	2 (22%)
2	ADP	B	501	-	28,29,29	1.39	4 (14%)	43,45,45	1.92	12 (27%)
2	ADP	E	501	-	28,29,29	1.37	4 (14%)	43,45,45	1.88	10 (23%)
3	P3S	D	502	-	11,14,14	2.00	3 (27%)	9,21,21	5.88	3 (33%)
2	ADP	J	501	-	28,29,29	1.42	4 (14%)	43,45,45	1.92	9 (20%)
2	ADP	D	501	-	28,29,29	1.38	4 (14%)	43,45,45	1.94	10 (23%)
2	ADP	U	501	-	28,29,29	1.49	5 (17%)	43,45,45	1.85	8 (18%)
3	P3S	O	502	-	11,14,14	1.84	3 (27%)	9,21,21	6.90	3 (33%)
3	P3S	Q	502	-	11,14,14	1.94	3 (27%)	9,21,21	6.87	3 (33%)
2	ADP	O	501	-	28,29,29	1.41	4 (14%)	43,45,45	1.90	11 (25%)
3	P3S	U	502	-	11,14,14	1.92	3 (27%)	9,21,21	7.96	4 (44%)
2	ADP	Q	501	-	28,29,29	1.48	5 (17%)	43,45,45	1.87	9 (20%)
3	P3S	E	502	-	11,14,14	2.04	3 (27%)	9,21,21	6.86	4 (44%)
3	P3S	S	502	-	11,14,14	2.07	3 (27%)	9,21,21	6.54	3 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	S	501	-	-	2/16/32/32	0/3/3/3
3	P3S	J	502	-	-	5/9/16/16	-
3	P3S	M	502	-	-	6/9/16/16	-
2	ADP	A	501	-	-	6/16/32/32	0/3/3/3
3	P3S	A	502	-	-	5/9/16/16	-
3	P3S	H	502	-	-	6/9/16/16	-
2	ADP	H	501	-	-	4/16/32/32	0/3/3/3
3	P3S	B	502	-	-	5/9/16/16	-
2	ADP	M	501	-	-	7/16/32/32	0/3/3/3
2	ADP	W	501	-	-	3/16/32/32	0/3/3/3
3	P3S	W	502	-	-	4/9/16/16	-
2	ADP	B	501	-	-	5/16/32/32	0/3/3/3
2	ADP	E	501	-	-	1/16/32/32	0/3/3/3
3	P3S	D	502	-	-	7/9/16/16	-
2	ADP	J	501	-	-	2/16/32/32	0/3/3/3
2	ADP	D	501	-	-	2/16/32/32	0/3/3/3
2	ADP	U	501	-	-	7/16/32/32	0/3/3/3
3	P3S	O	502	-	-	7/9/16/16	-
3	P3S	Q	502	-	-	8/9/16/16	-
2	ADP	O	501	-	-	2/16/32/32	0/3/3/3
3	P3S	U	502	-	-	5/9/16/16	-
2	ADP	Q	501	-	-	3/16/32/32	0/3/3/3
3	P3S	E	502	-	-	6/9/16/16	-
3	P3S	S	502	-	-	8/9/16/16	-

The worst 5 of 84 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	U	501	ADP	C5-C4	4.88	1.47	1.39
2	W	501	ADP	C5-C4	4.85	1.47	1.39
2	Q	501	ADP	C5-C4	4.78	1.47	1.39
2	B	501	ADP	C5-C4	4.75	1.47	1.39
2	M	501	ADP	C5-C4	4.73	1.47	1.39

The worst 5 of 152 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	P3S	OE-SD-CE	-22.46	73.59	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	502	P3S	OE-SD-CE	-22.17	74.06	109.21
3	U	502	P3S	OE-SD-CE	-21.42	75.25	109.21
3	J	502	P3S	OE-SD-CE	-20.74	76.32	109.21
3	H	502	P3S	OE-SD-CE	-19.19	78.77	109.21

There are no chirality outliers.

5 of 116 torsion outliers are listed below:

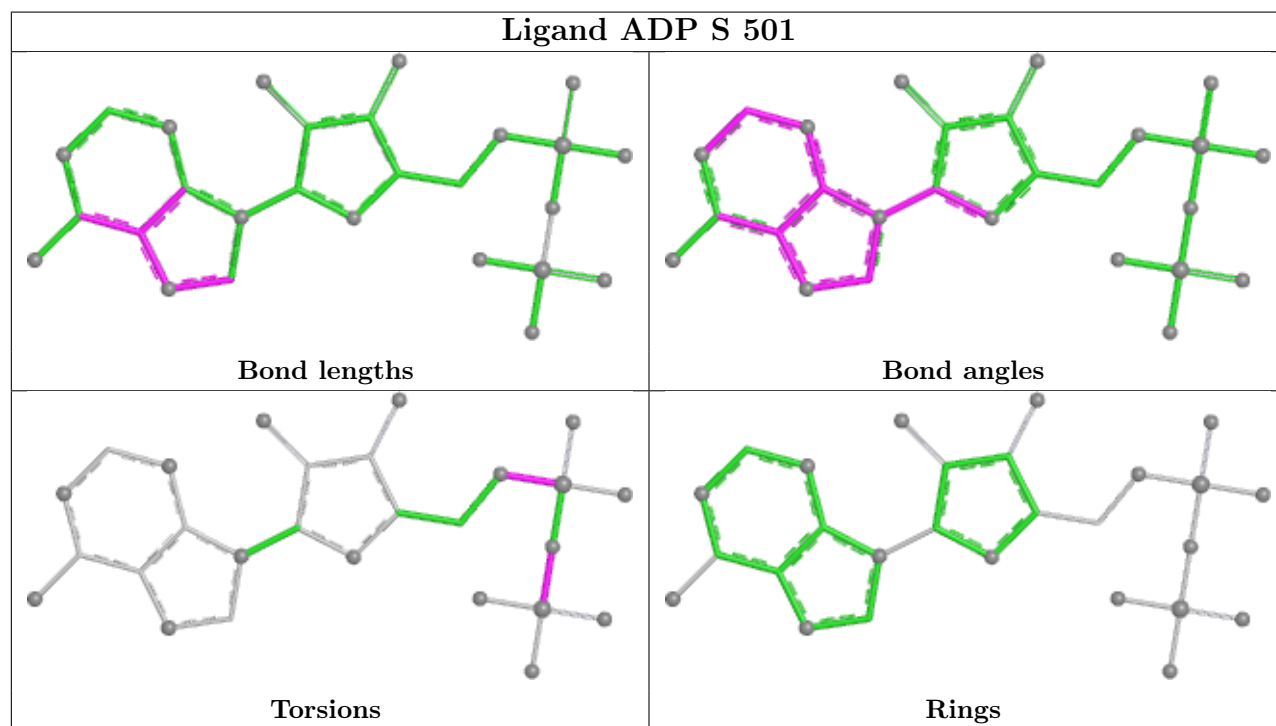
Mol	Chain	Res	Type	Atoms
2	A	501	ADP	C5'-O5'-PA-O1A
2	A	501	ADP	C5'-O5'-PA-O3A
2	B	501	ADP	C5'-O5'-PA-O1A
2	B	501	ADP	C5'-O5'-PA-O2A
2	B	501	ADP	C5'-O5'-PA-O3A

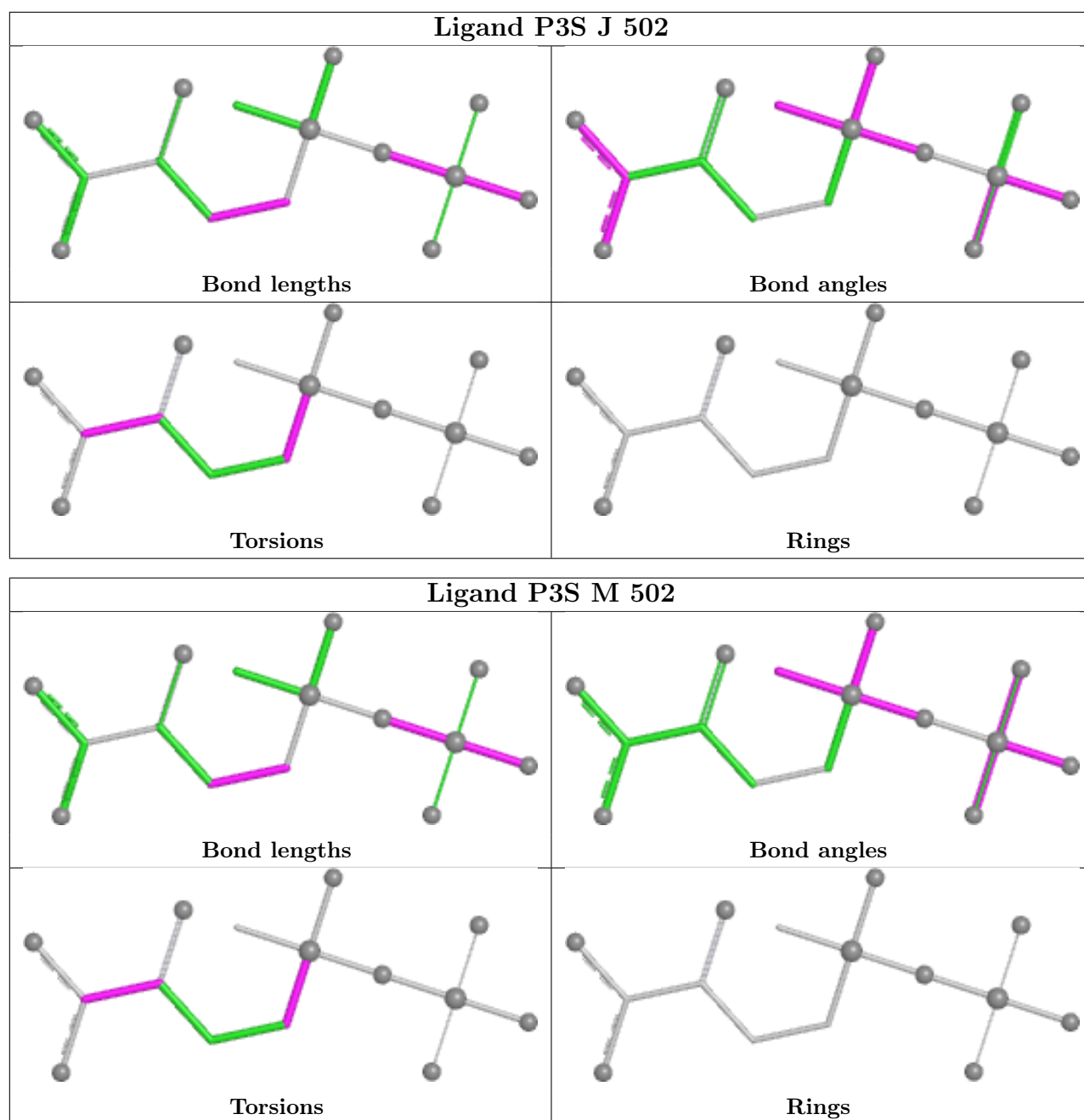
There are no ring outliers.

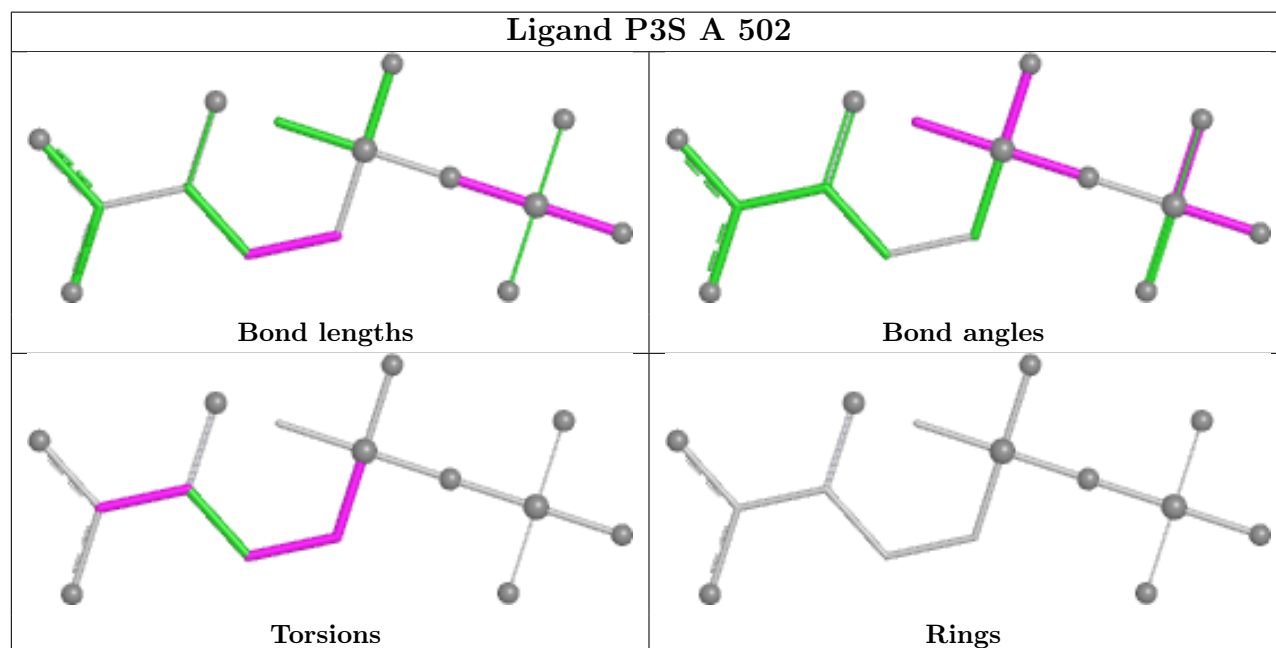
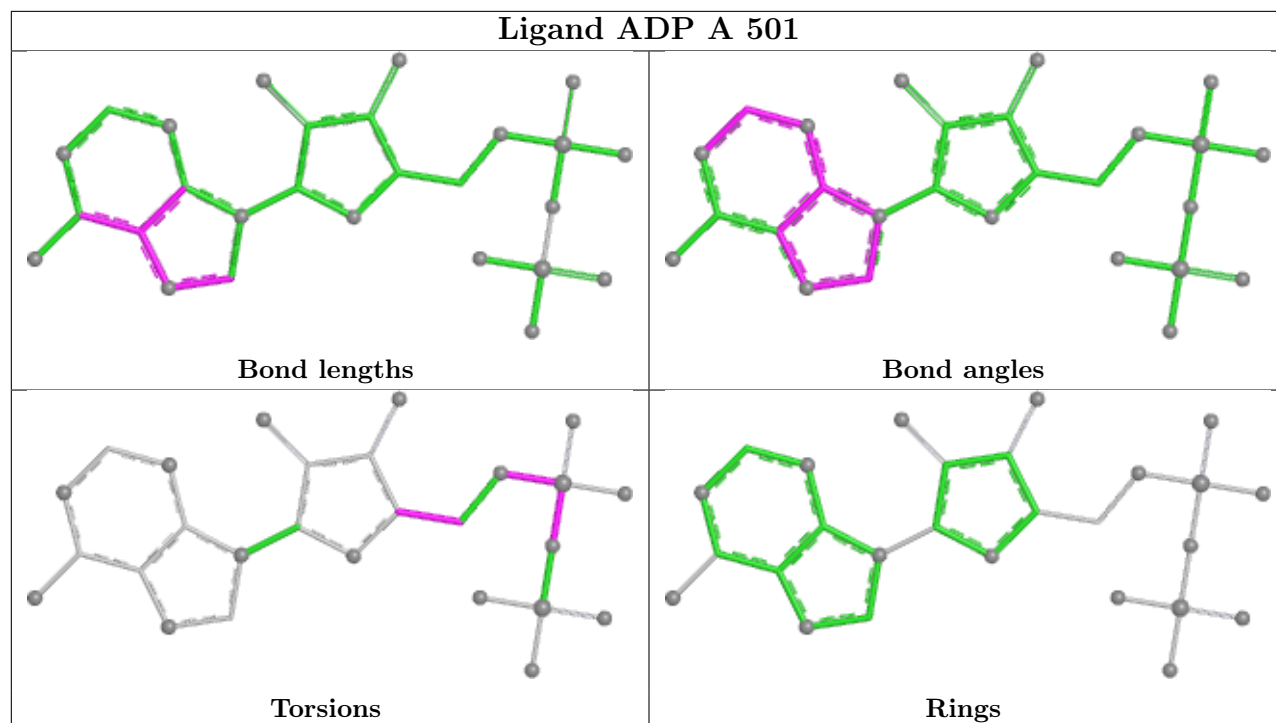
22 monomers are involved in 60 short contacts:

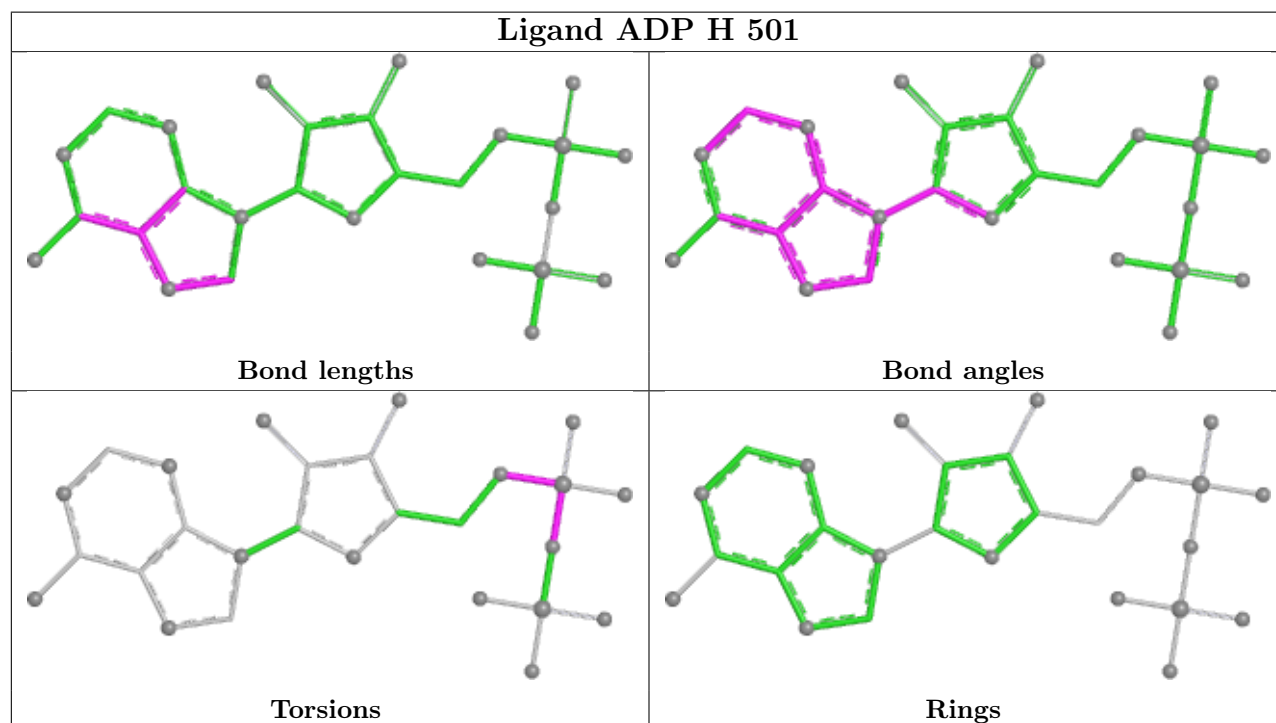
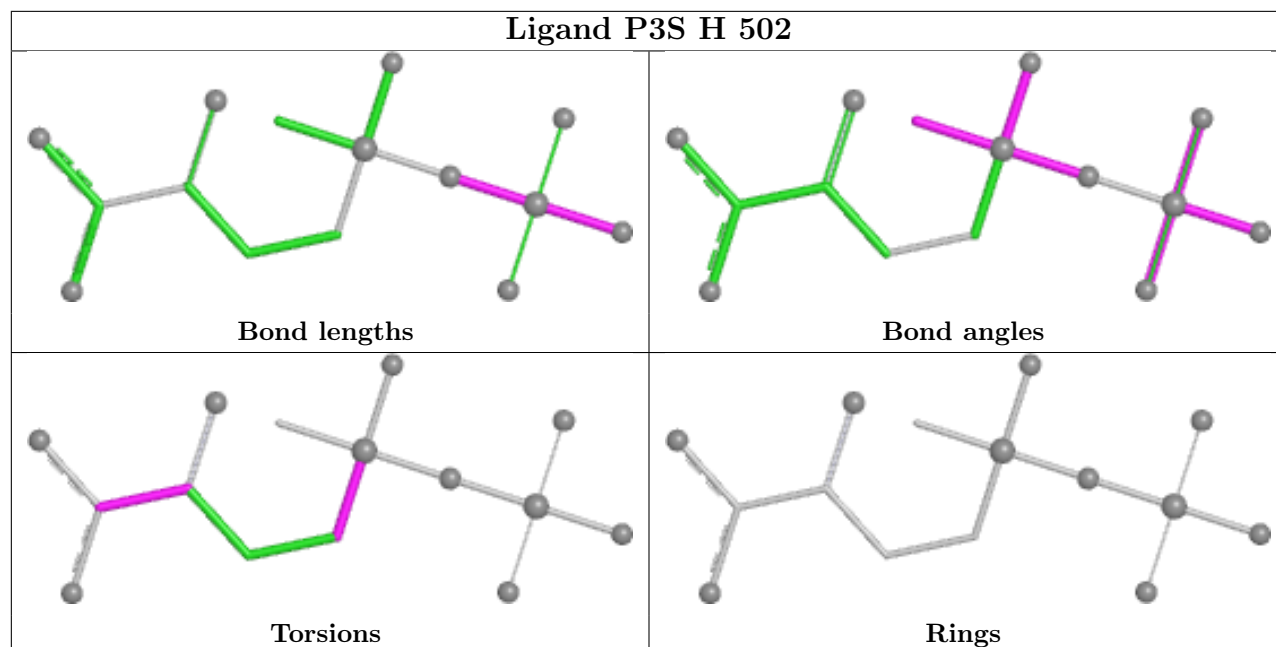
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	S	501	ADP	2	0
3	J	502	P3S	1	0
3	M	502	P3S	5	0
2	A	501	ADP	5	0
3	A	502	P3S	1	0
3	H	502	P3S	2	0
2	H	501	ADP	3	0
3	B	502	P3S	4	0
2	M	501	ADP	3	0
2	B	501	ADP	5	0
2	E	501	ADP	2	0
3	D	502	P3S	2	0
2	J	501	ADP	5	0
2	D	501	ADP	2	0
2	U	501	ADP	1	0
3	O	502	P3S	3	0
3	Q	502	P3S	1	0
2	O	501	ADP	4	0
3	U	502	P3S	5	0
2	Q	501	ADP	1	0
3	E	502	P3S	2	0
3	S	502	P3S	1	0

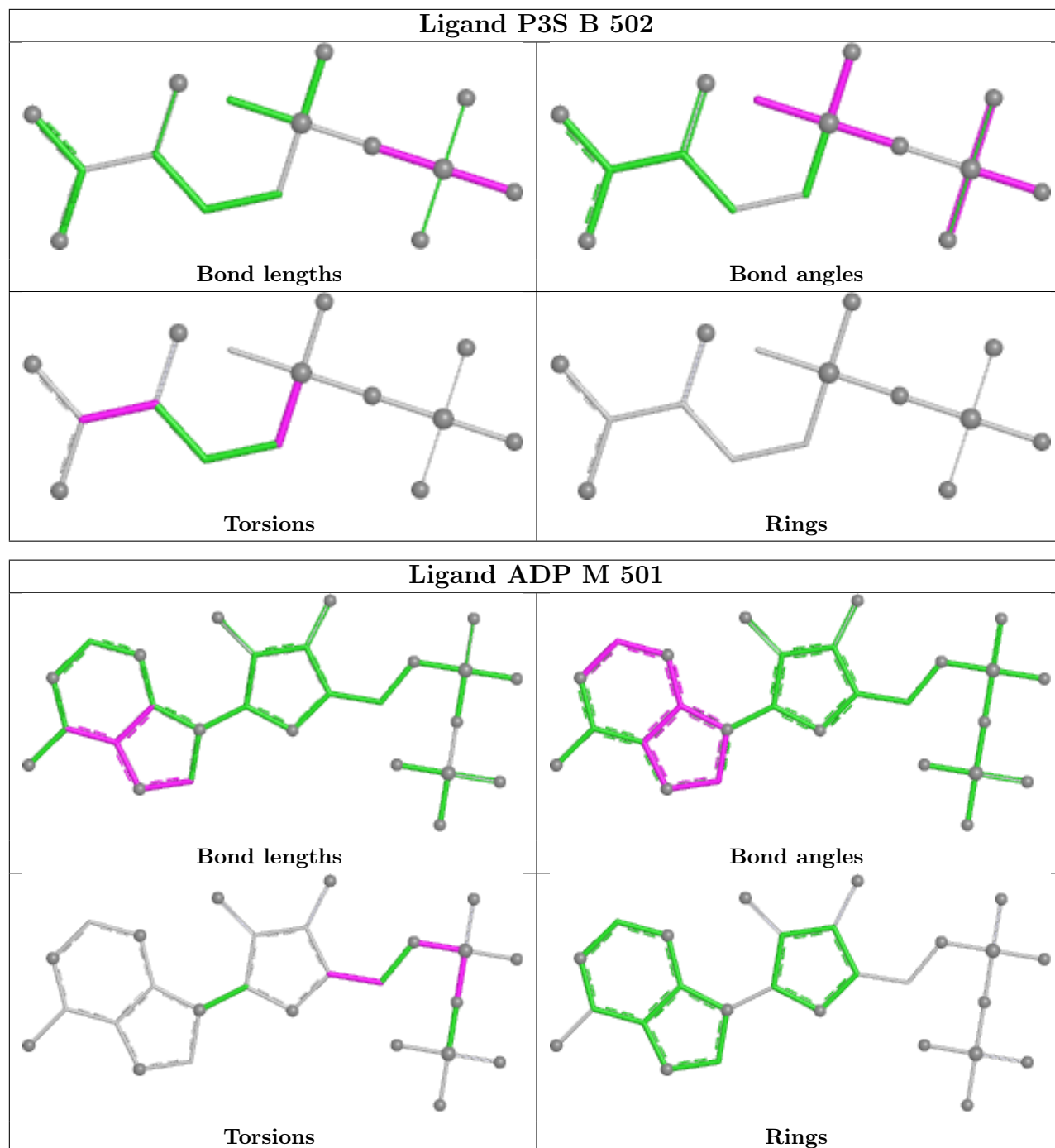
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

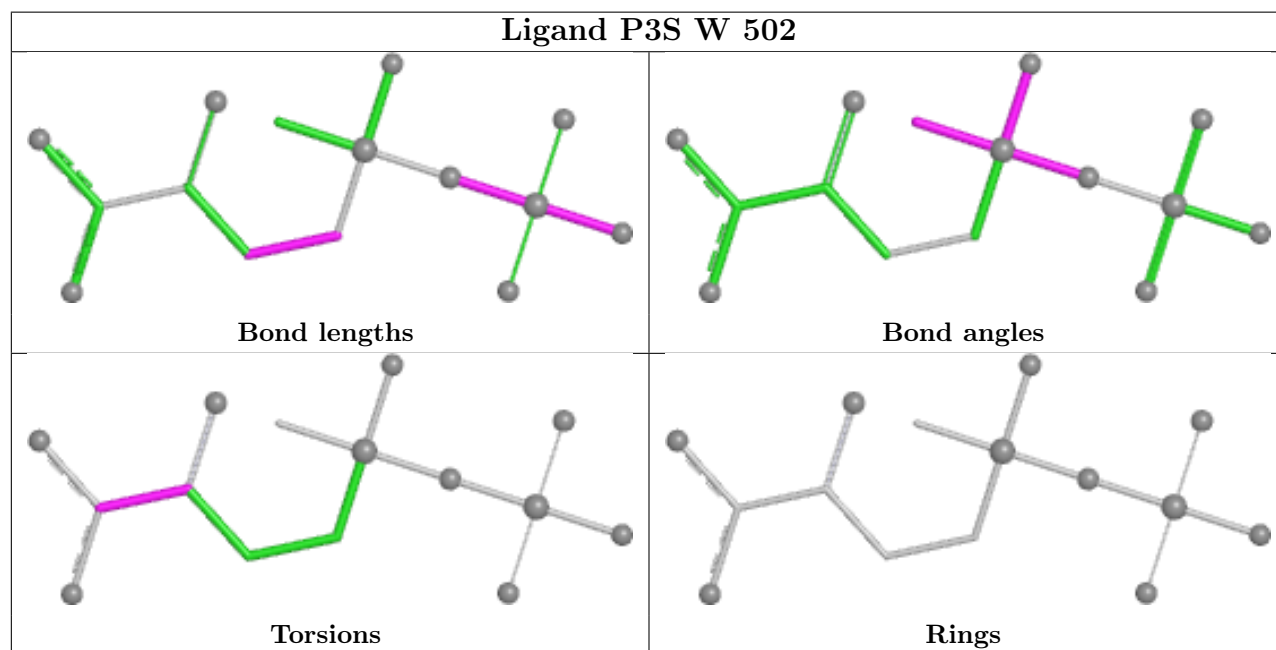
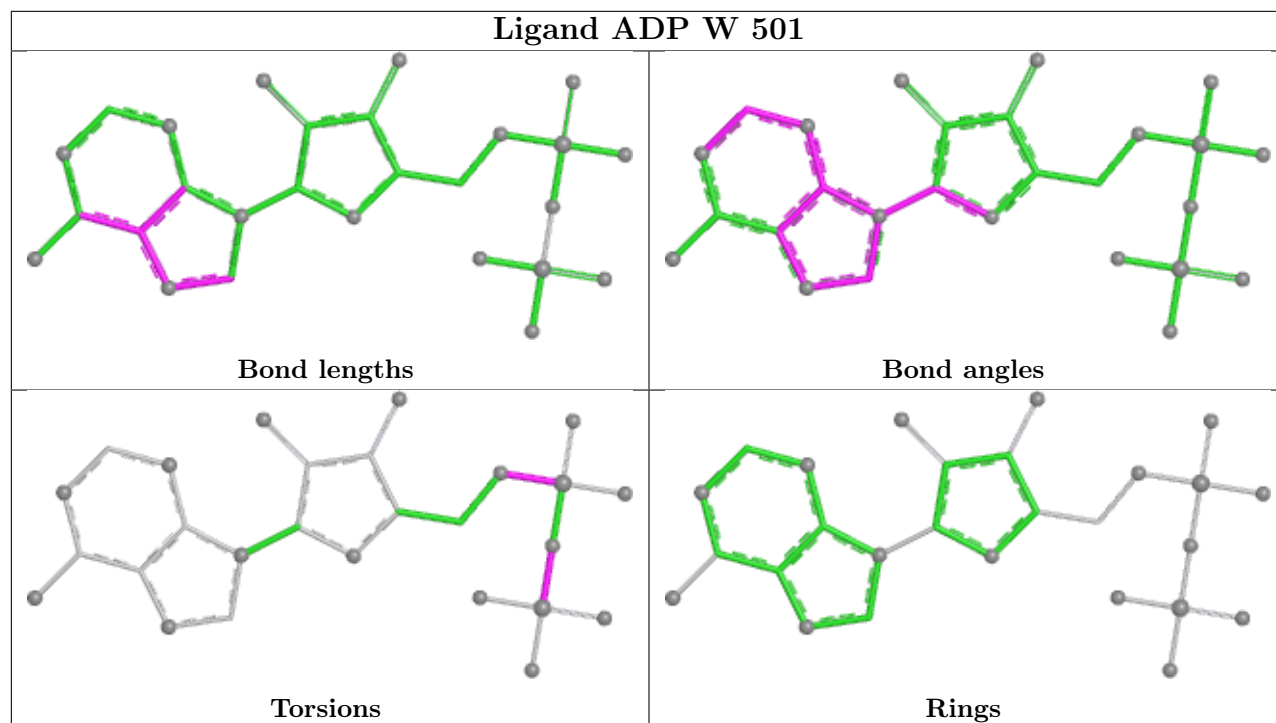


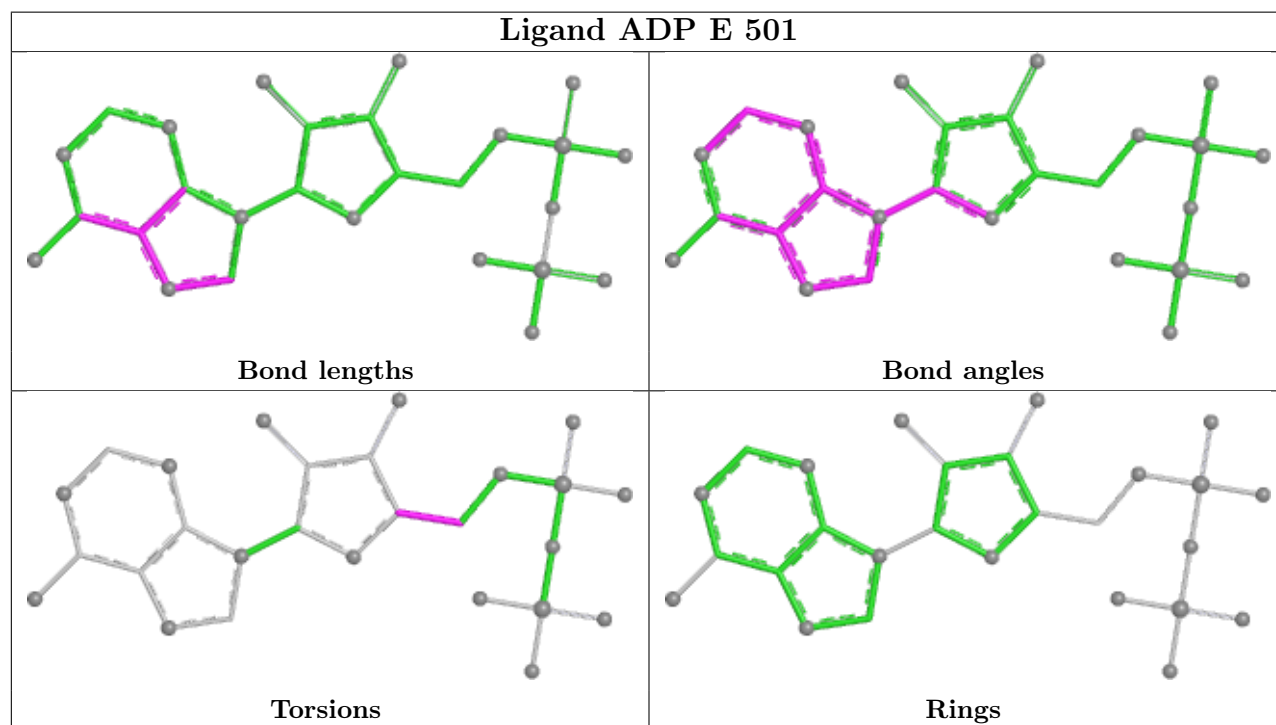
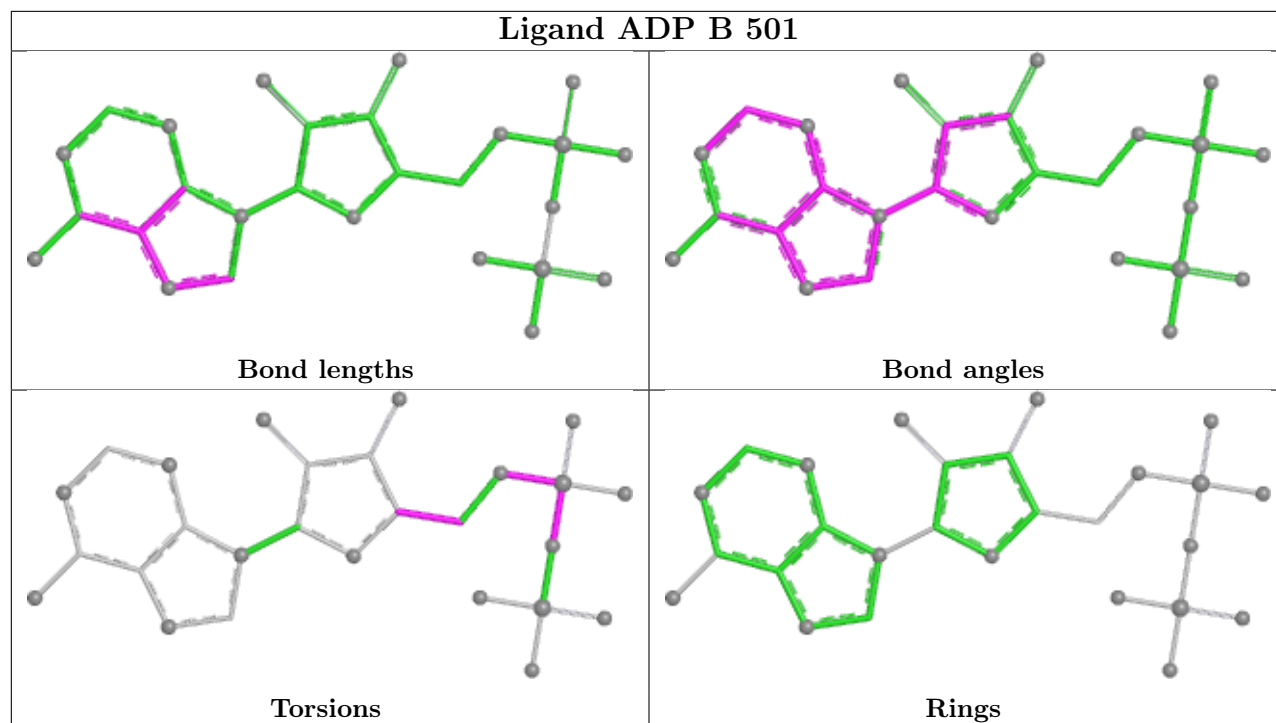


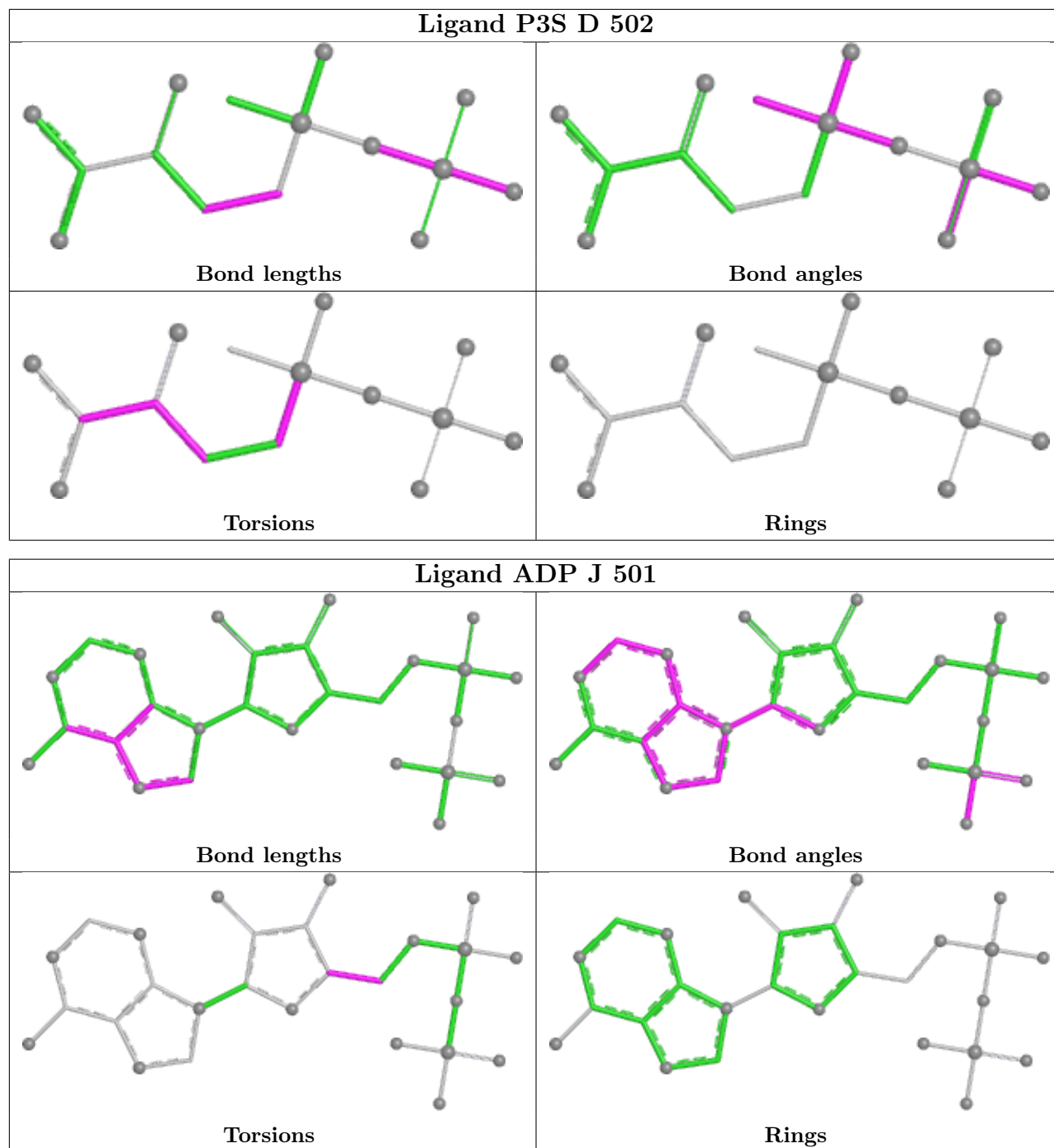


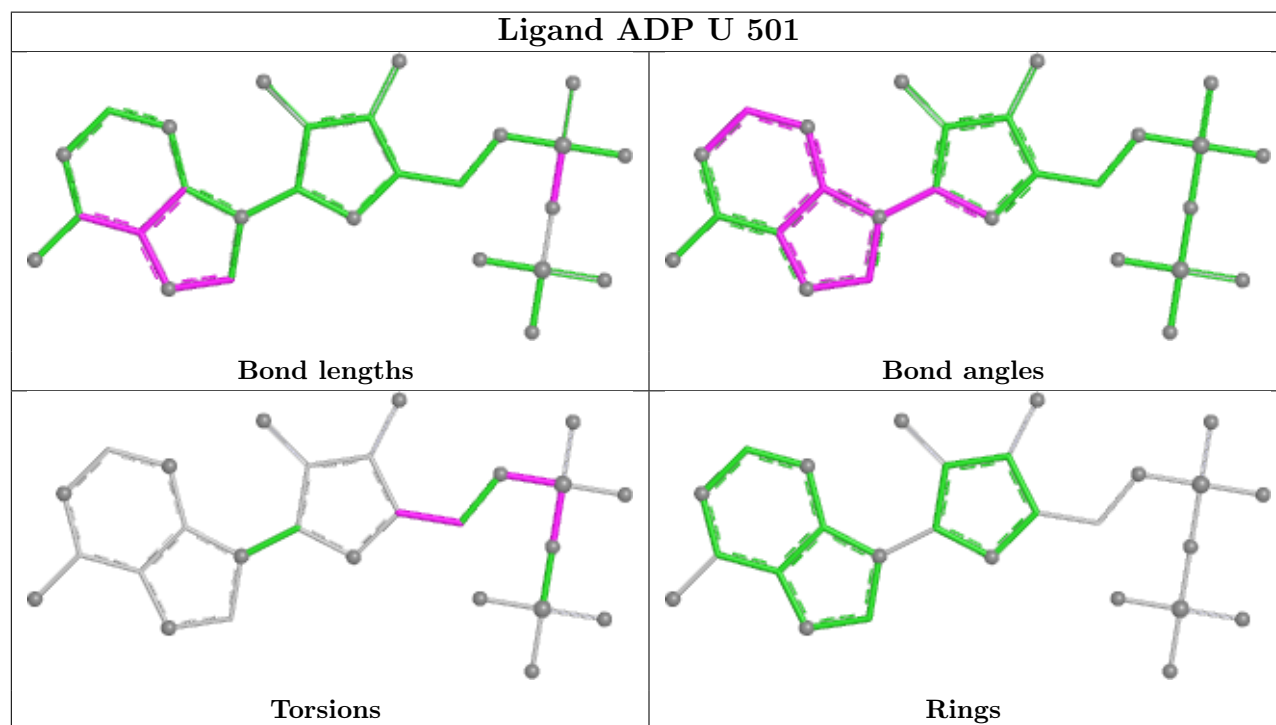
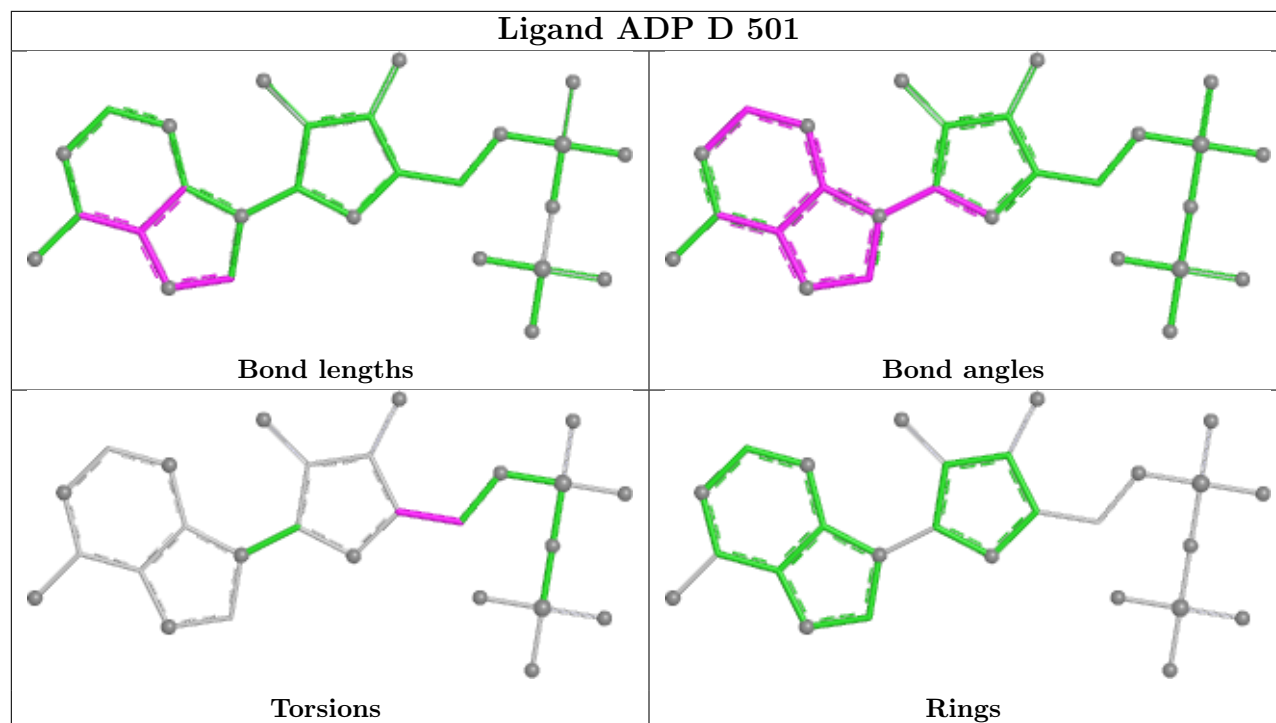


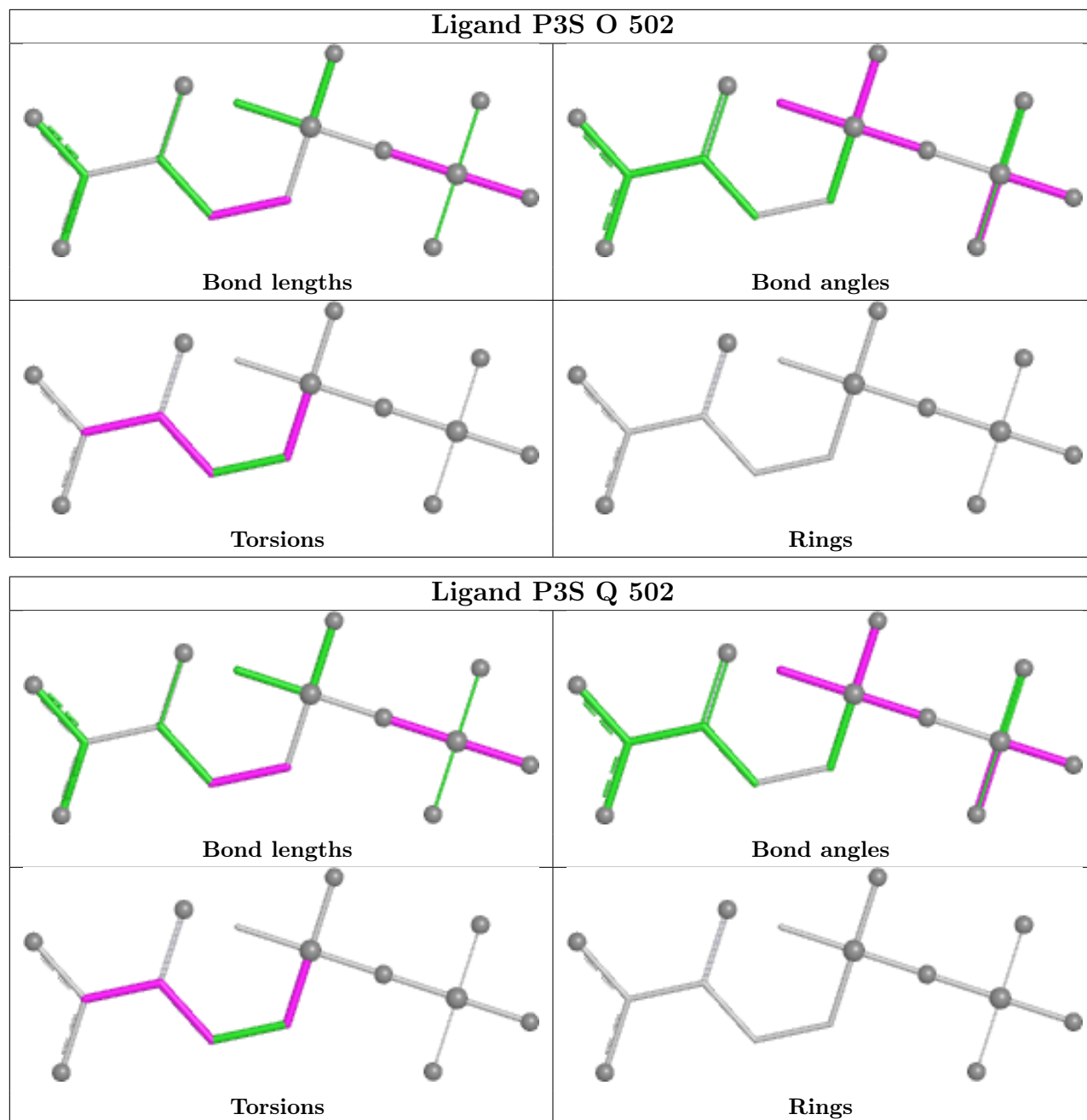


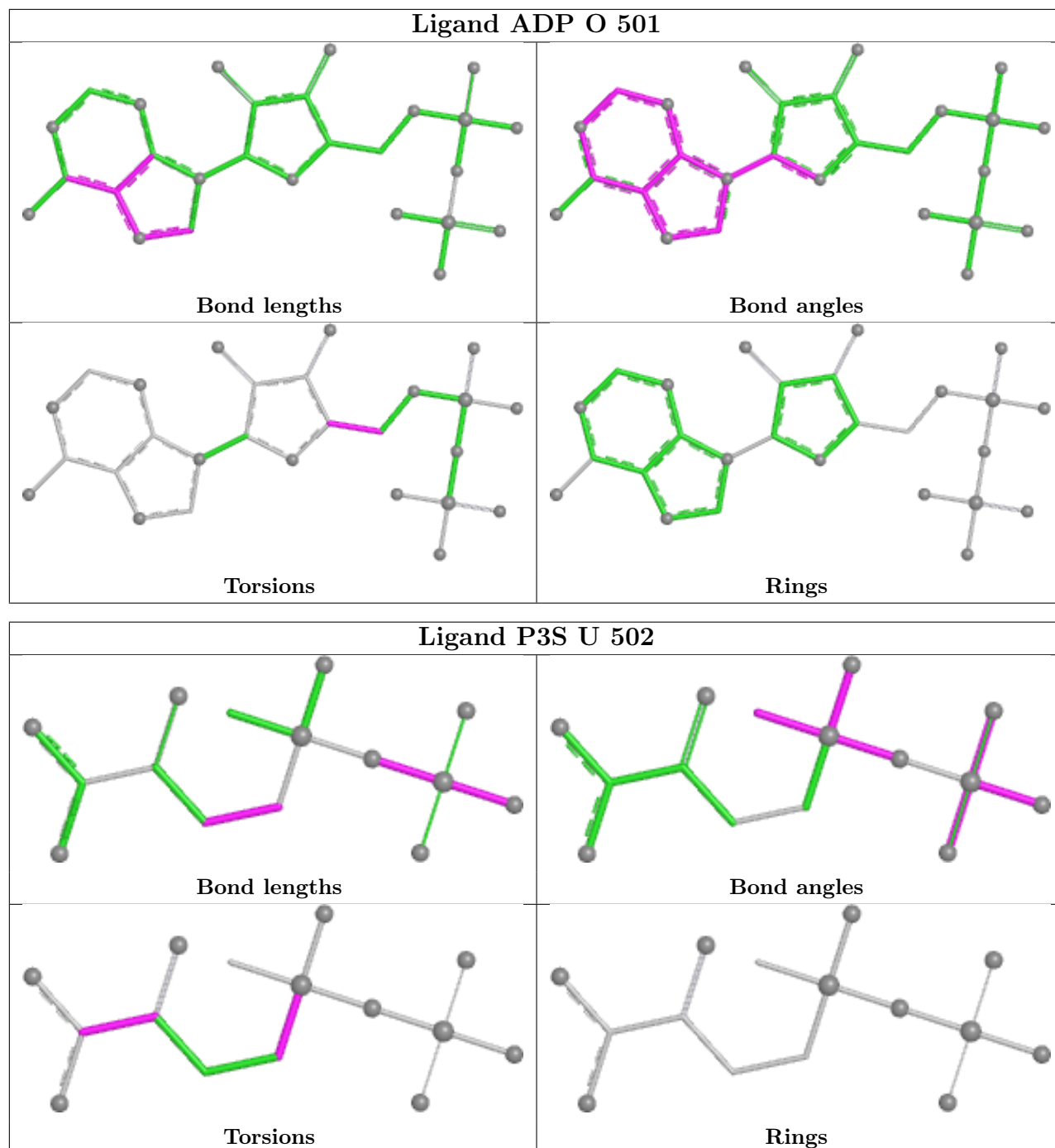


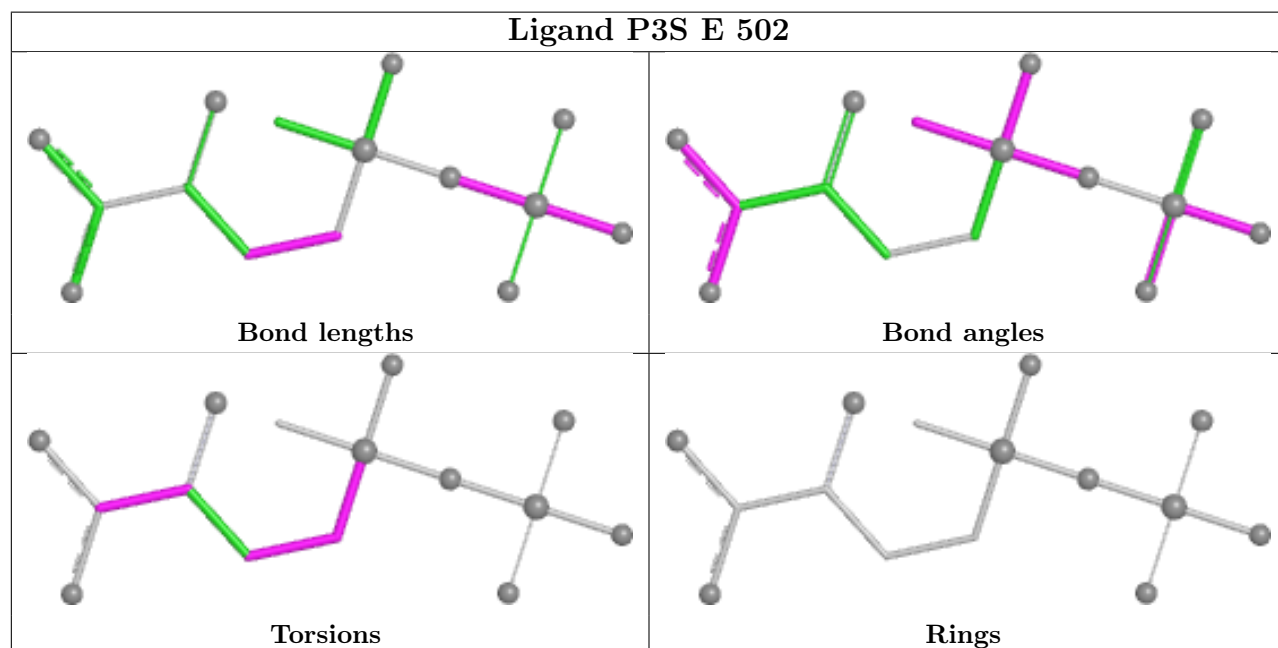
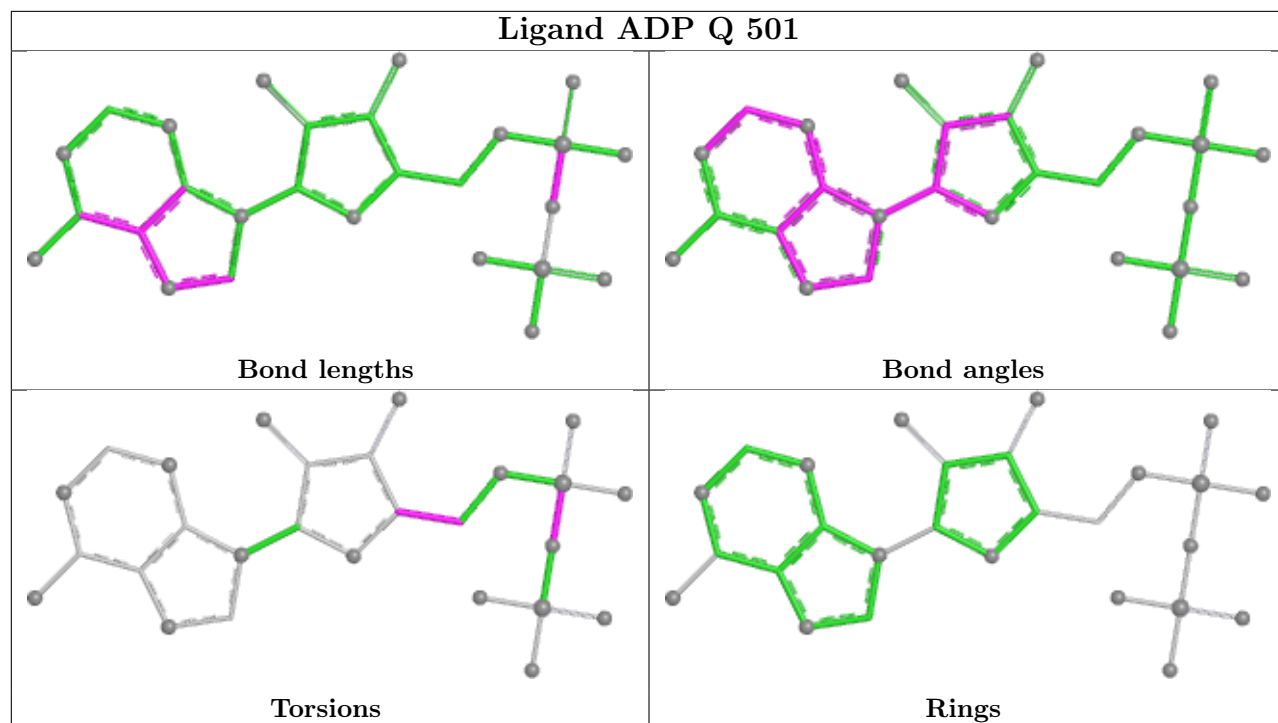


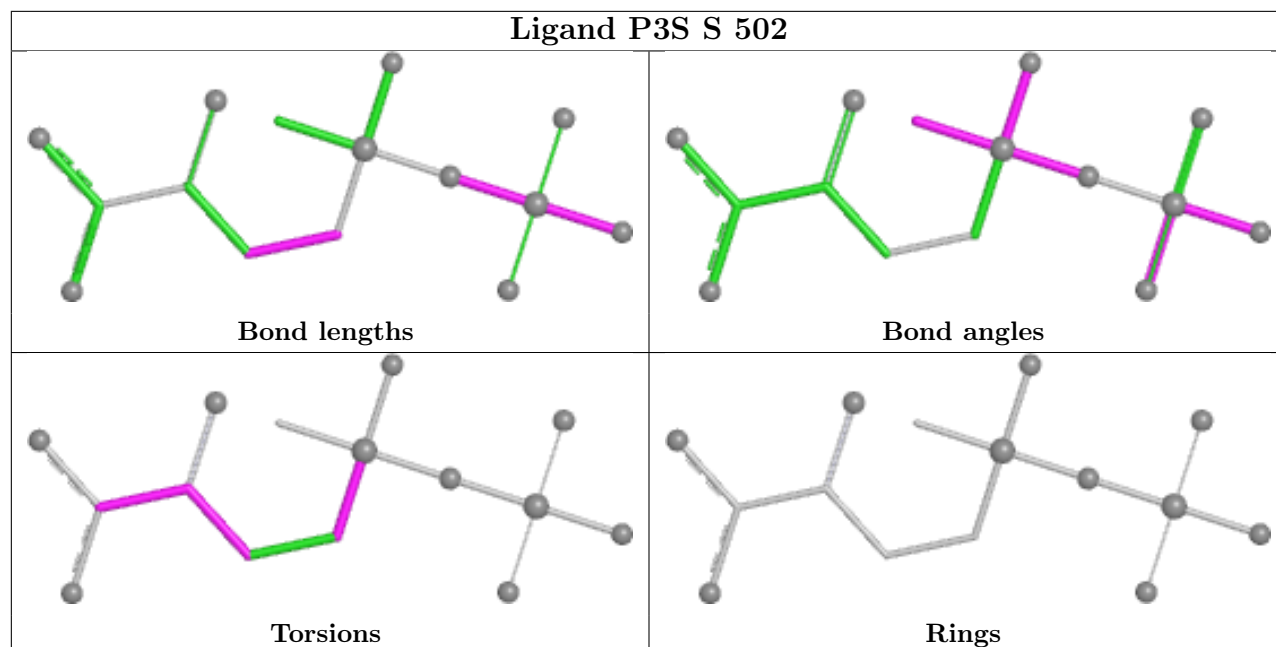












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	442/447 (98%)	-0.75	0 100 100	55, 100, 152, 201	0
1	B	442/447 (98%)	-0.72	0 100 100	56, 112, 163, 242	0
1	D	442/447 (98%)	-0.72	0 100 100	50, 102, 150, 228	0
1	E	442/447 (98%)	-0.74	0 100 100	56, 102, 152, 202	0
1	H	442/447 (98%)	-0.70	0 100 100	60, 104, 157, 234	0
1	J	442/447 (98%)	-0.70	0 100 100	64, 113, 172, 230	0
1	M	442/447 (98%)	-0.69	0 100 100	60, 116, 172, 207	0
1	O	442/447 (98%)	-0.68	0 100 100	46, 106, 163, 223	0
1	Q	442/447 (98%)	-0.67	0 100 100	56, 112, 162, 220	0
1	S	442/447 (98%)	-0.67	1 (0%) 91 82	66, 115, 170, 216	0
1	U	442/447 (98%)	-0.73	0 100 100	72, 121, 165, 257	0
1	W	442/447 (98%)	-0.68	0 100 100	70, 123, 181, 270	0
All	All	5304/5364 (98%)	-0.70	1 (0%) 100 100	46, 111, 166, 270	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	S	348	ALA	2.1

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands

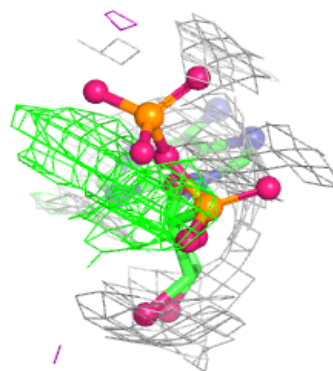
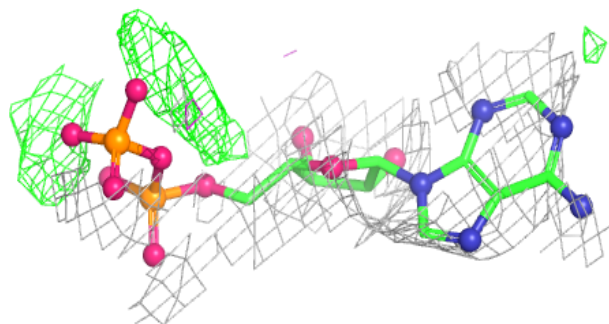
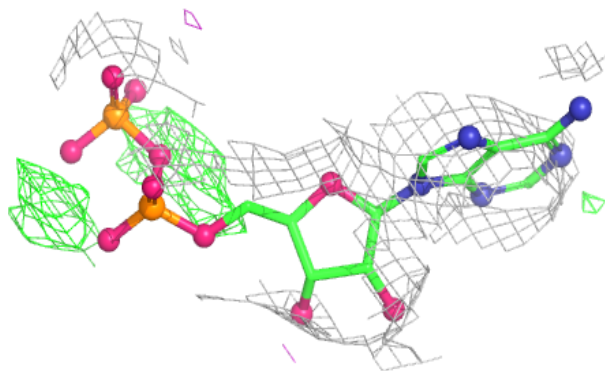
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	ADP	E	501	27/27	0.91	0.07	89,117,140,146	0
2	ADP	A	501	27/27	0.93	0.07	86,105,127,129	0
2	ADP	J	501	27/27	0.93	0.06	109,128,144,148	0
2	ADP	S	501	27/27	0.93	0.07	95,114,124,140	0
2	ADP	W	501	27/27	0.93	0.07	115,135,143,148	0
3	P3S	H	502	15/15	0.94	0.06	90,100,114,117	0
3	P3S	S	502	15/15	0.94	0.08	98,114,120,123	0
2	ADP	O	501	27/27	0.95	0.06	84,91,114,118	0
2	ADP	Q	501	27/27	0.95	0.06	94,111,116,121	0
2	ADP	D	501	27/27	0.95	0.06	80,97,112,117	0
2	ADP	U	501	27/27	0.95	0.07	102,122,141,154	0
2	ADP	H	501	27/27	0.95	0.07	92,107,122,127	0
3	P3S	D	502	15/15	0.95	0.09	72,80,107,118	0
2	ADP	B	501	27/27	0.95	0.05	83,97,112,119	0
3	P3S	Q	502	15/15	0.95	0.06	86,93,116,125	0
2	ADP	M	501	27/27	0.95	0.07	101,119,131,136	0
3	P3S	E	502	15/15	0.96	0.06	91,96,118,118	0
3	P3S	B	502	15/15	0.96	0.06	83,97,112,116	0
3	P3S	U	502	15/15	0.96	0.05	101,110,122,125	0
3	P3S	W	502	15/15	0.96	0.07	95,101,121,122	0
3	P3S	A	502	15/15	0.97	0.06	82,88,100,104	0
3	P3S	J	502	15/15	0.97	0.05	86,91,108,109	0
3	P3S	M	502	15/15	0.97	0.06	82,88,95,96	0
3	P3S	O	502	15/15	0.97	0.07	73,82,109,109	0

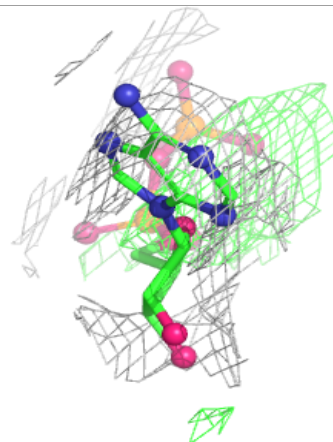
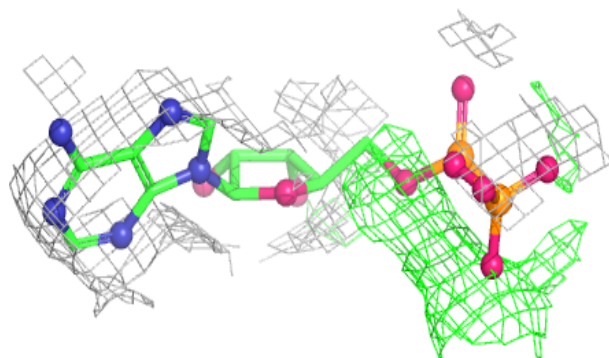
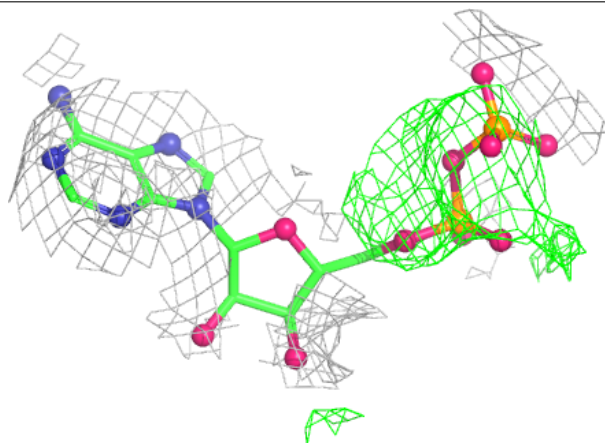
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around ADP E 501:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

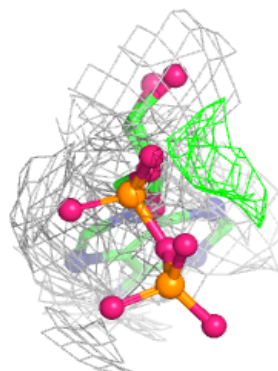
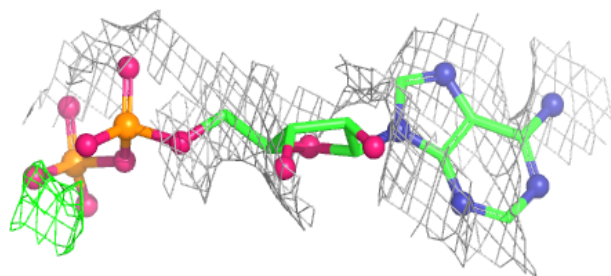
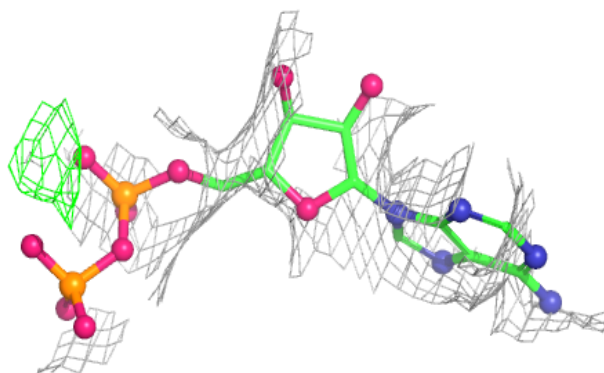
**Electron density around ADP A 501:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

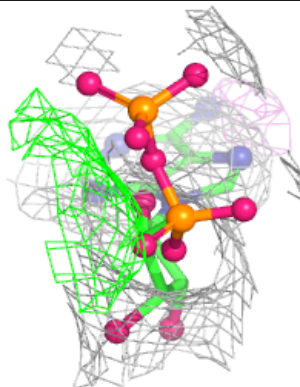
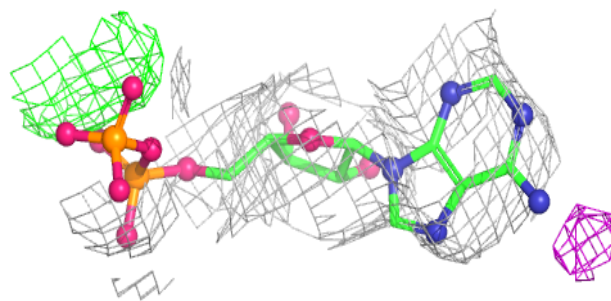
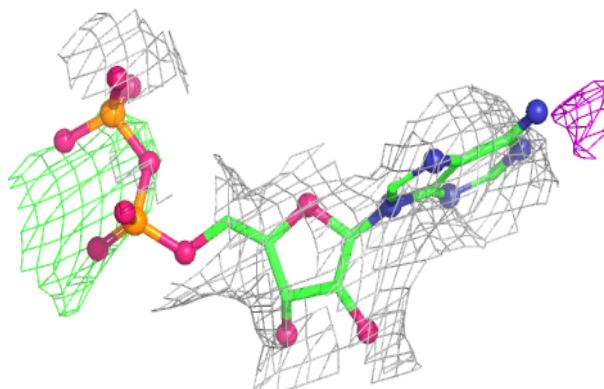


**Electron density around ADP J 501:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

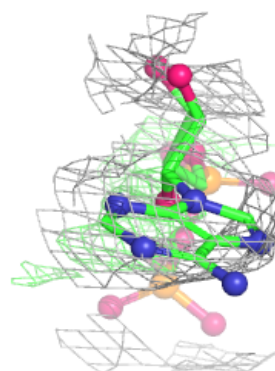
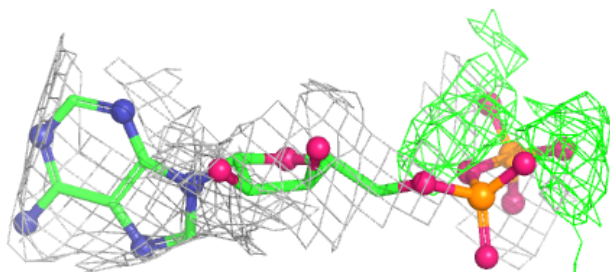
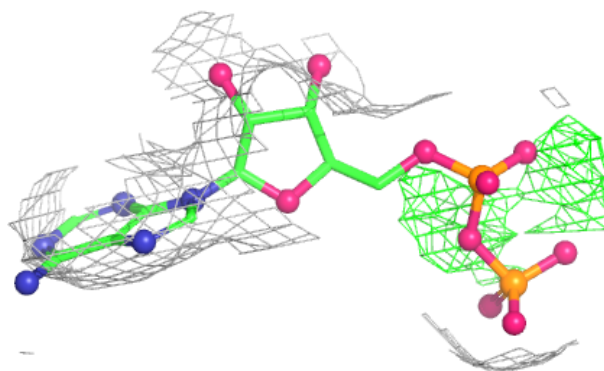
**Electron density around ADP S 501:**

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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

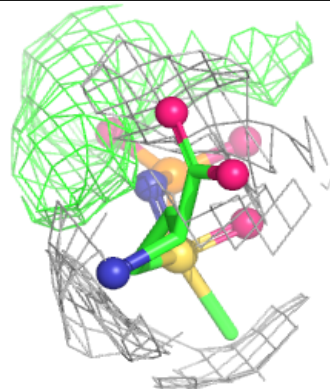
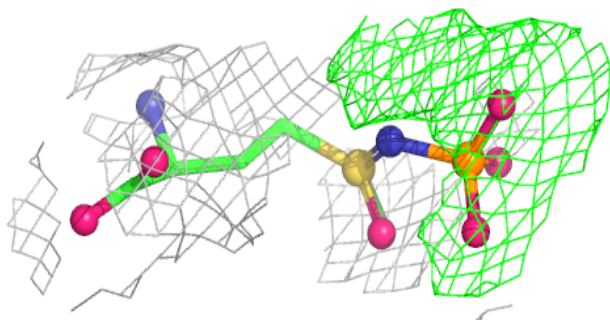
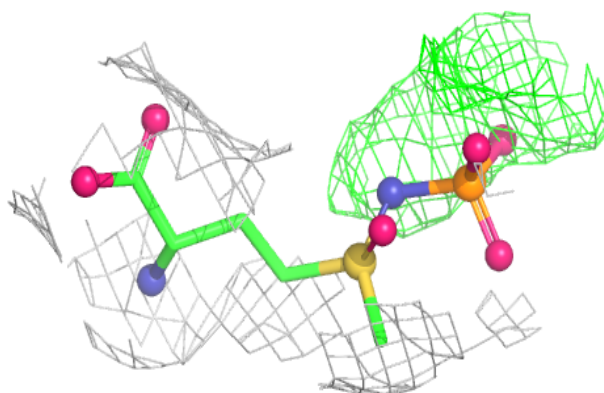


**Electron density around ADP W 501:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

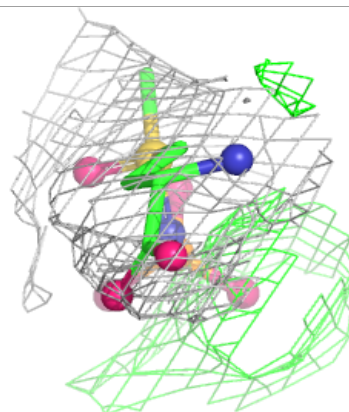
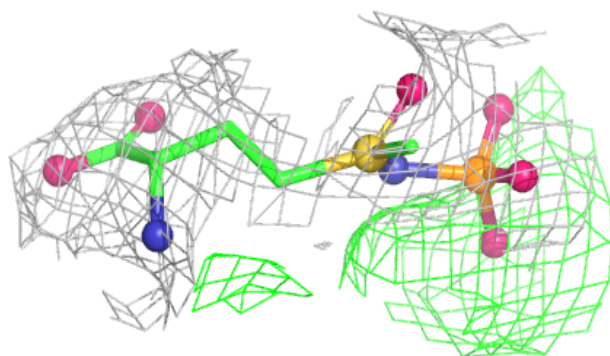
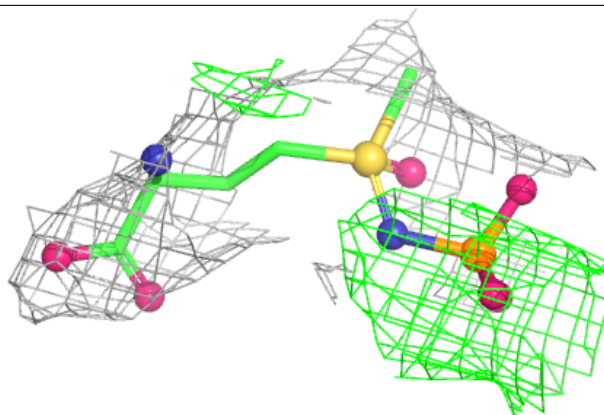
**Electron density around P3S H 502:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

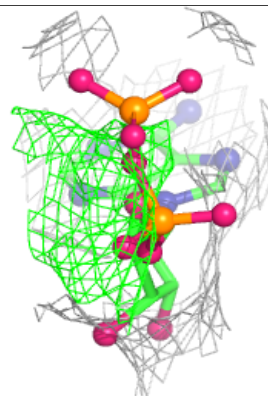
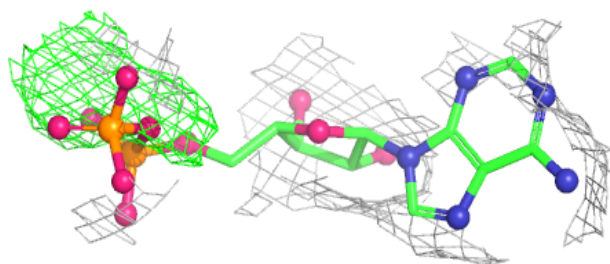
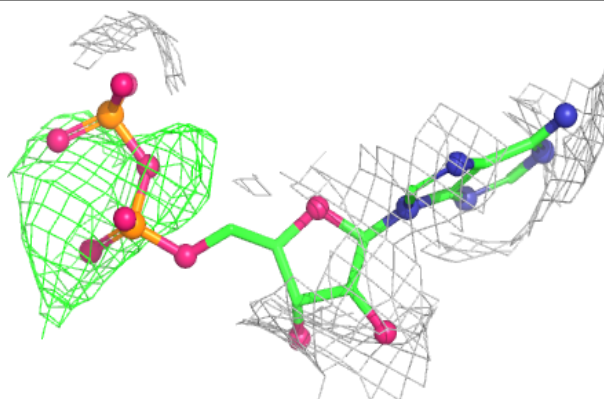


**Electron density around P3S S 502:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

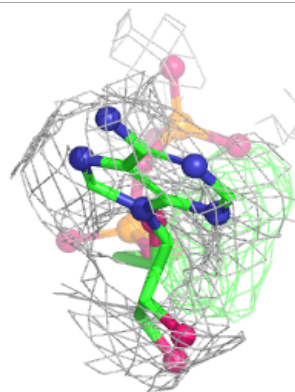
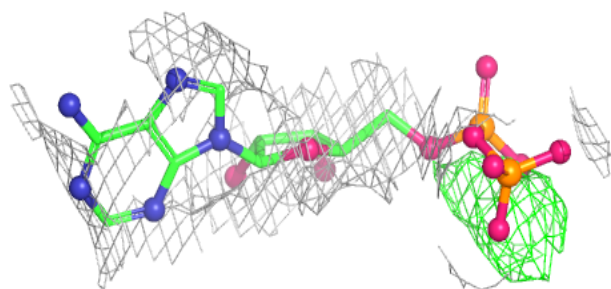
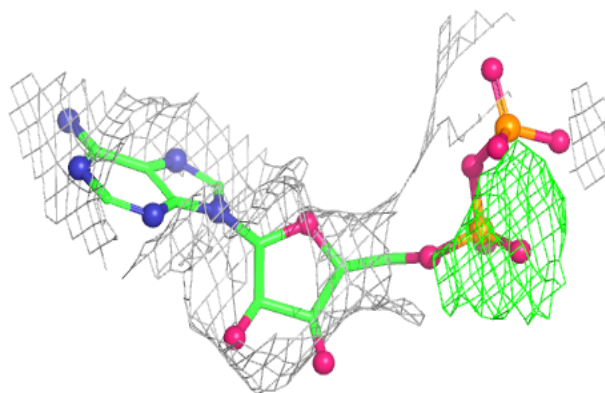
**Electron density around ADP O 501:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

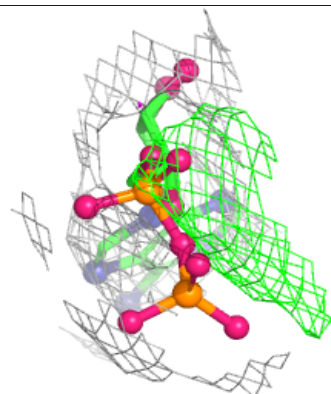
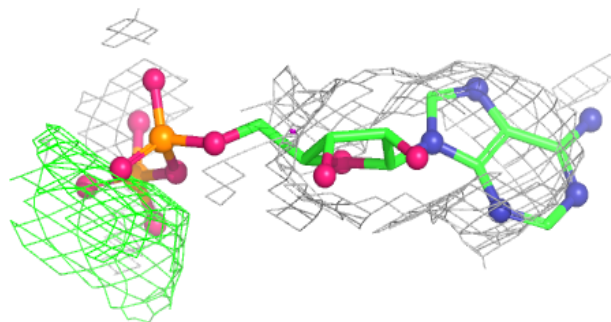
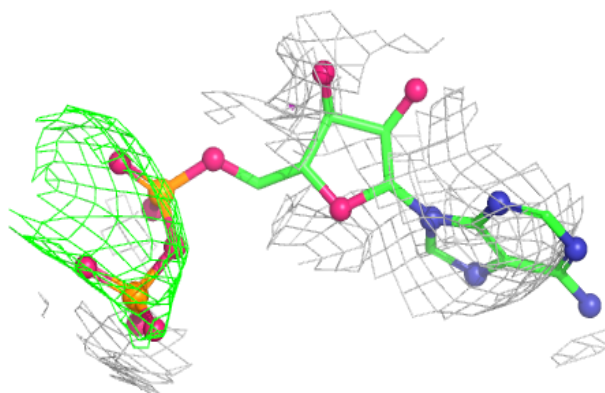


**Electron density around ADP Q 501:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

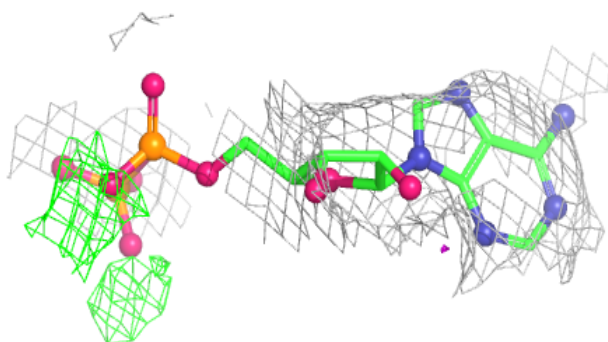
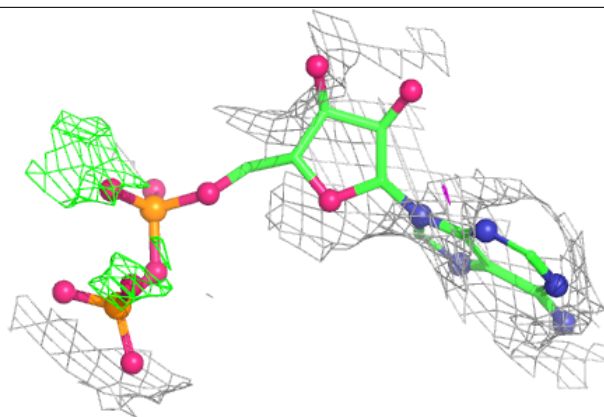
**Electron density around ADP D 501:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

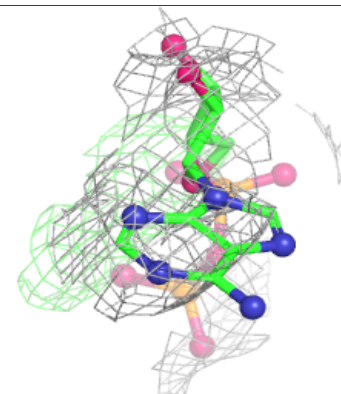
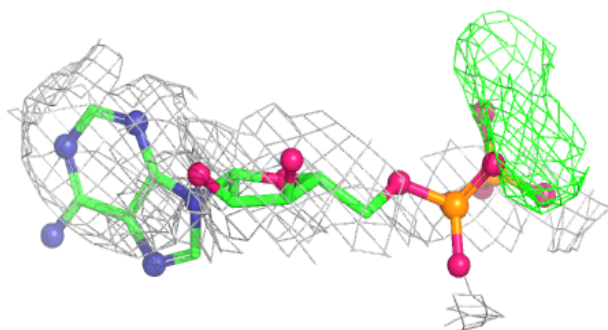
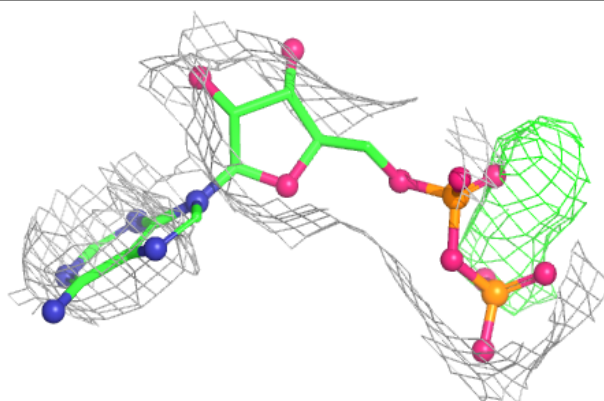


**Electron density around ADP U 501:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

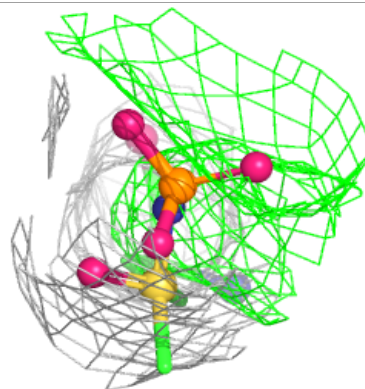
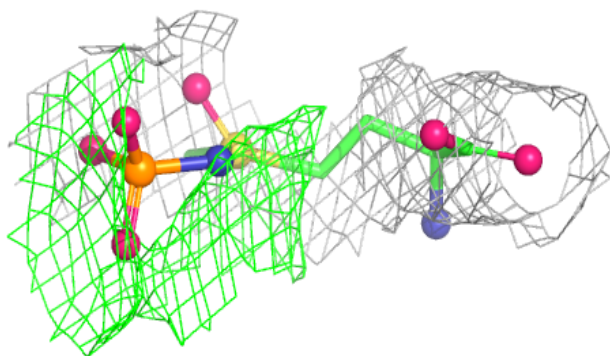
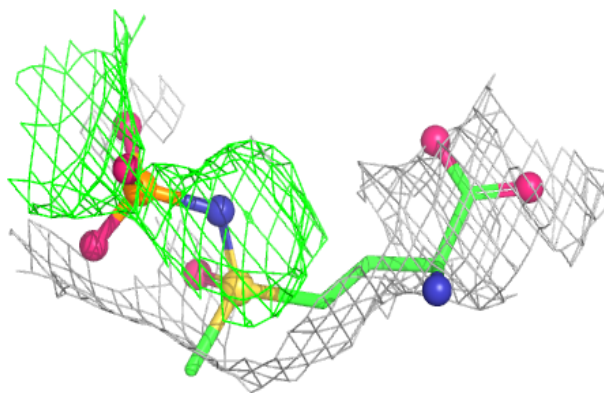
**Electron density around ADP H 501:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

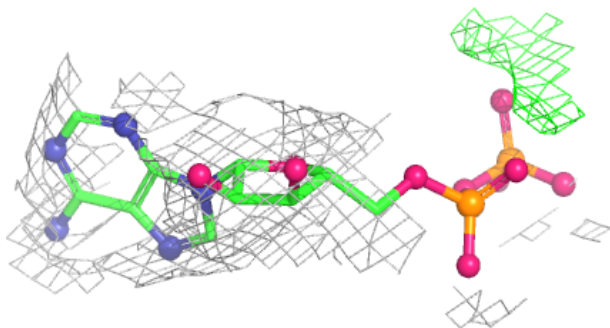
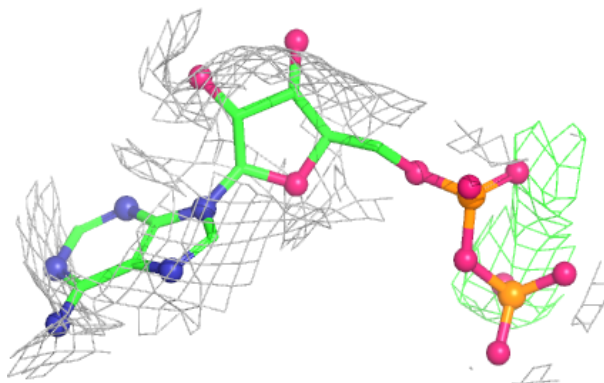


**Electron density around P3S D 502:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

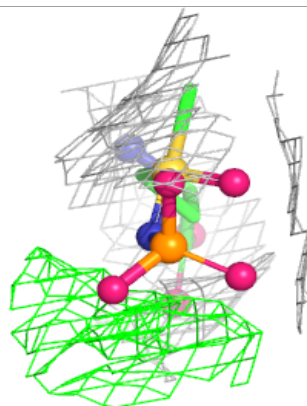
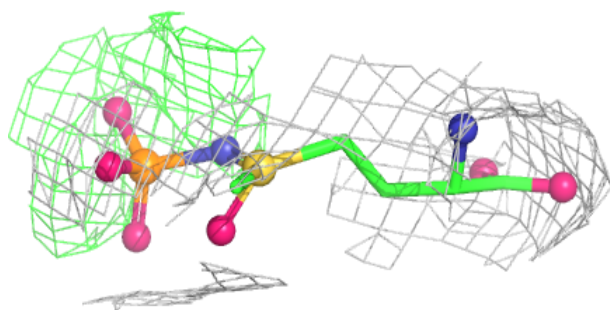
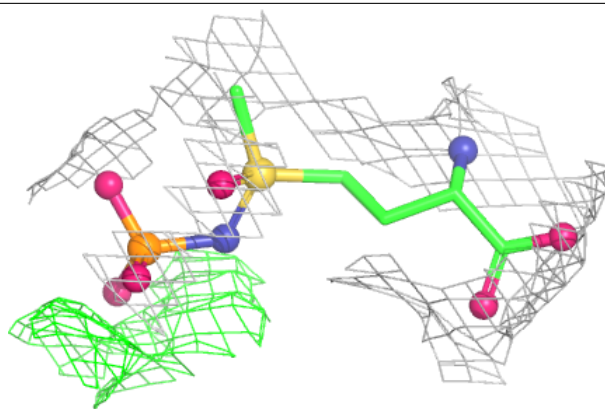
**Electron density around ADP B 501:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

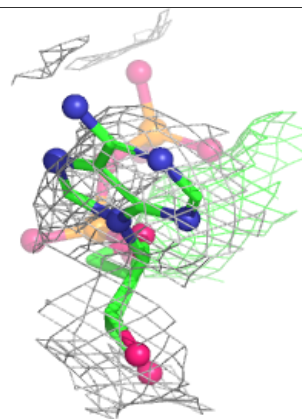
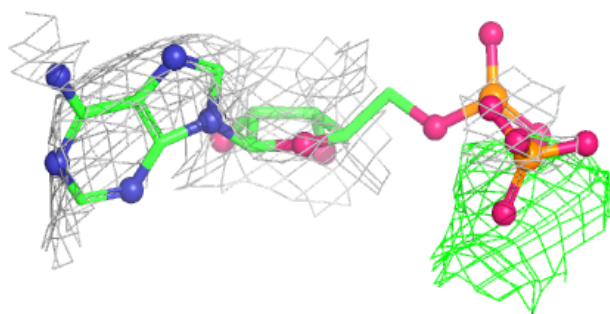
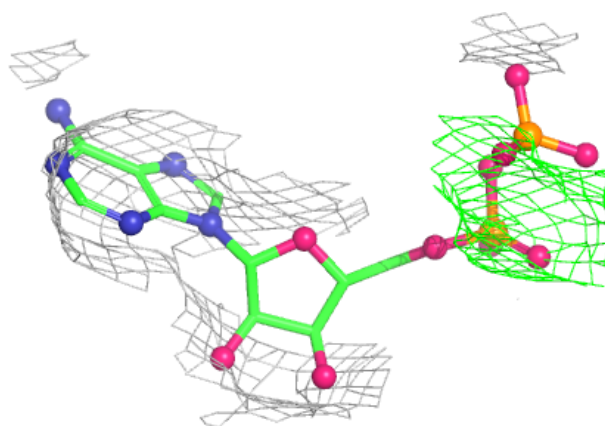


**Electron density around P3S Q 502:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

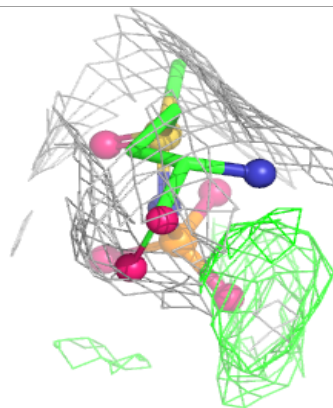
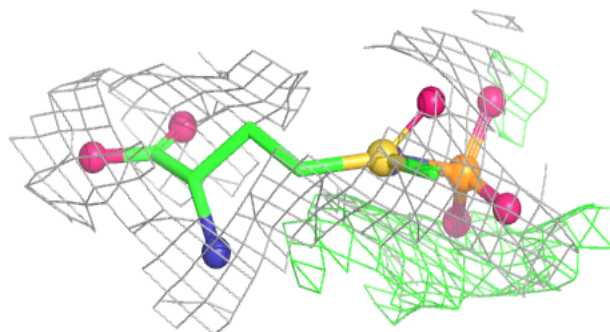
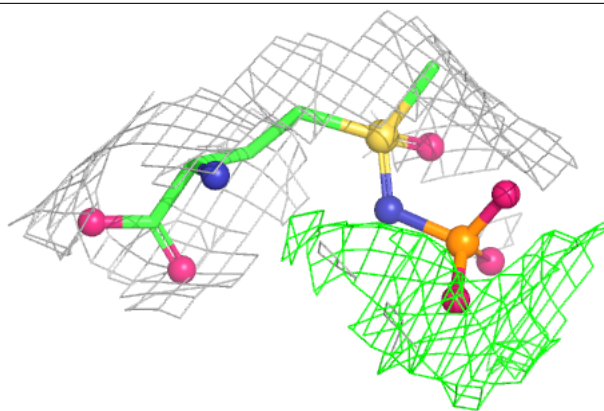
**Electron density around ADP M 501:**

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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



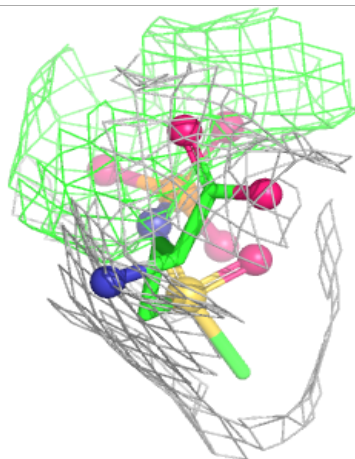
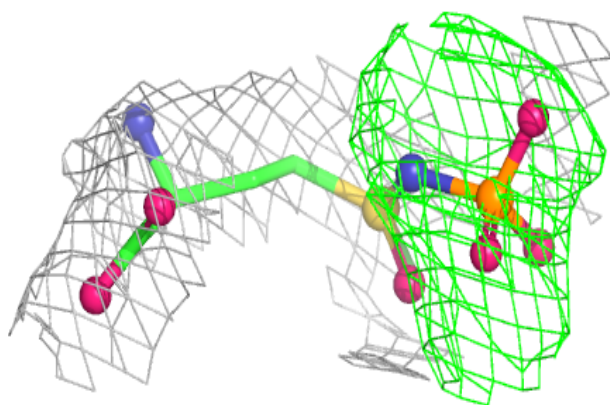
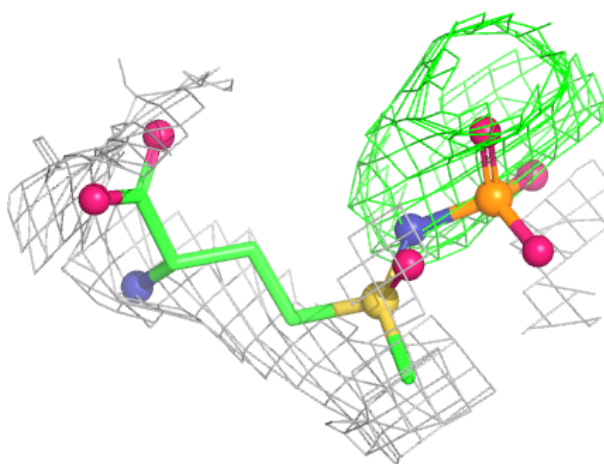
**Electron density around P3S E 502:**

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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



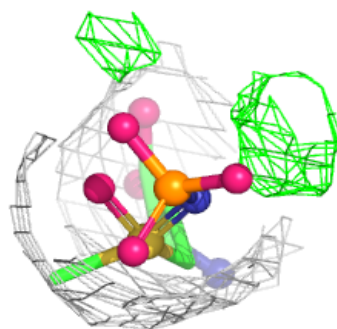
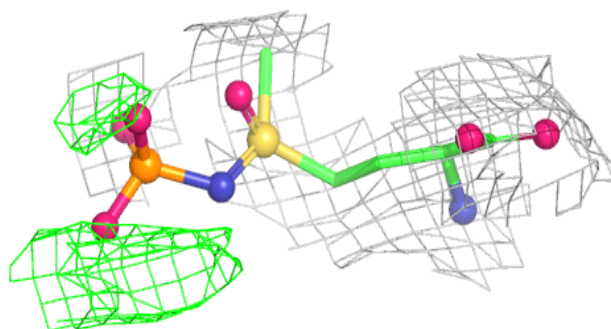
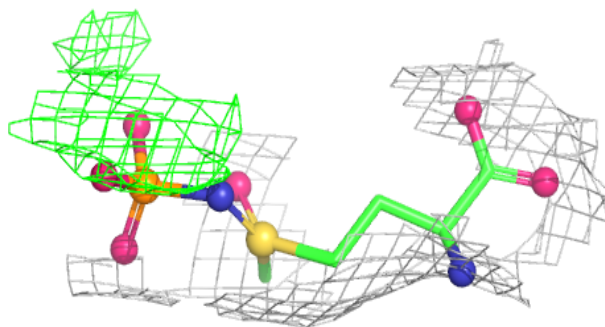
**Electron density around P3S B 502:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
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and green (positive)

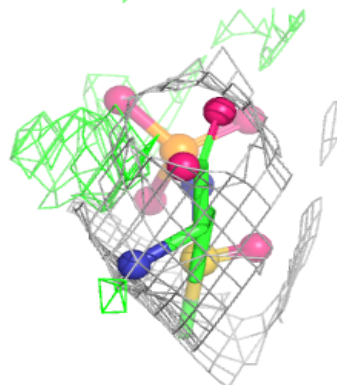
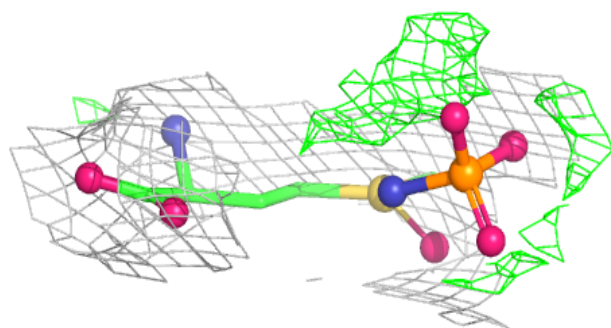
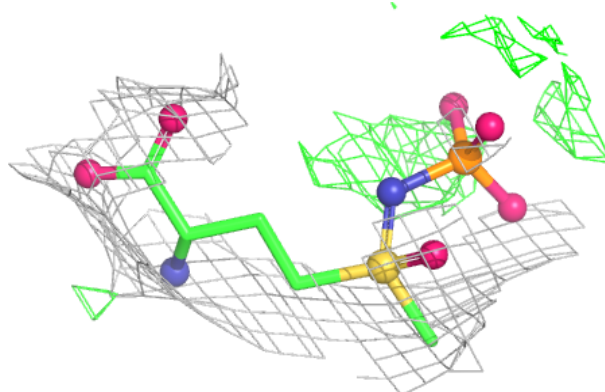


**Electron density around P3S U 502:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

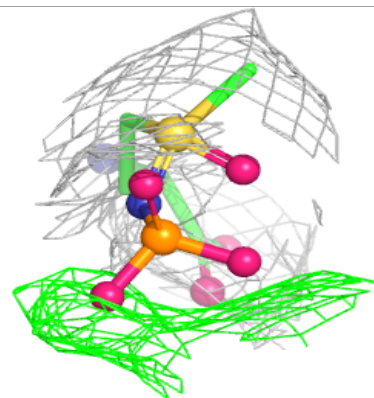
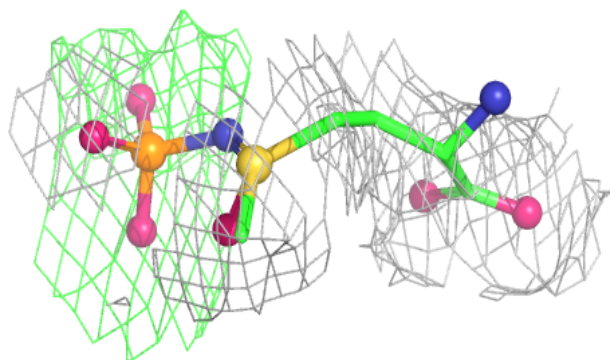
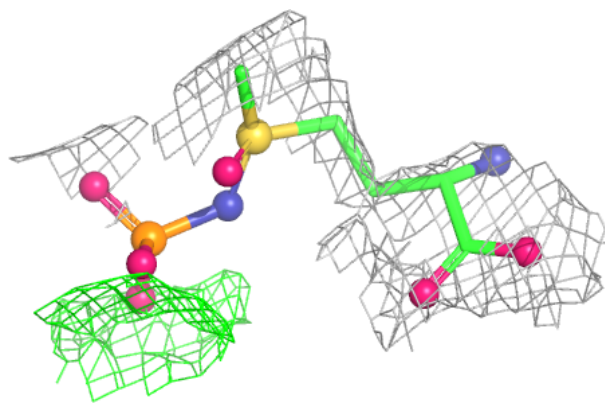
**Electron density around P3S W 502:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
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and green (positive)

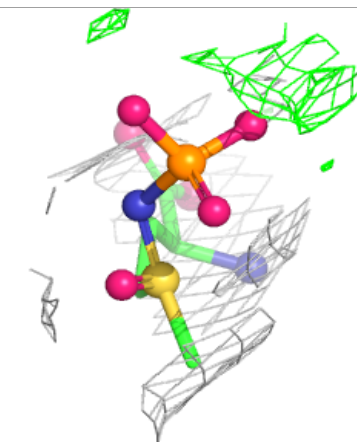
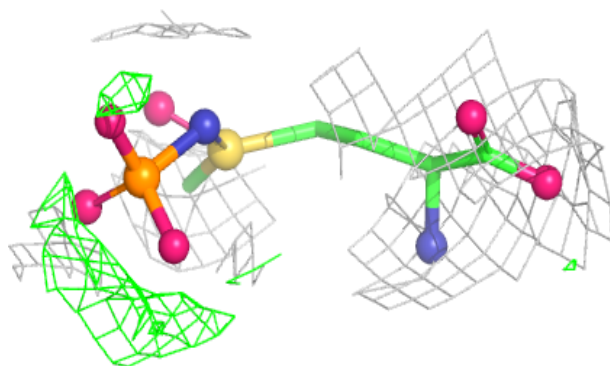
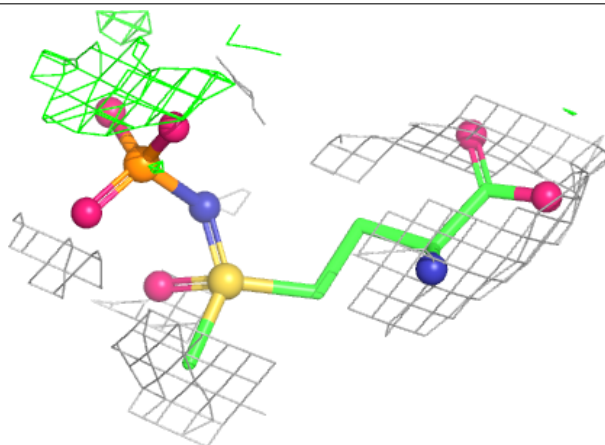


**Electron density around P3S A 502:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
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and green (positive)

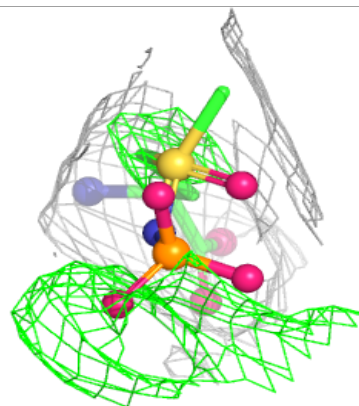
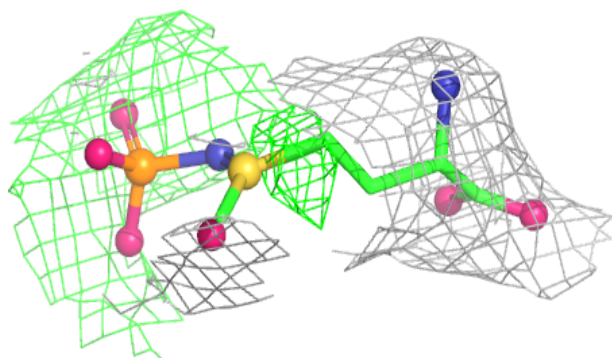
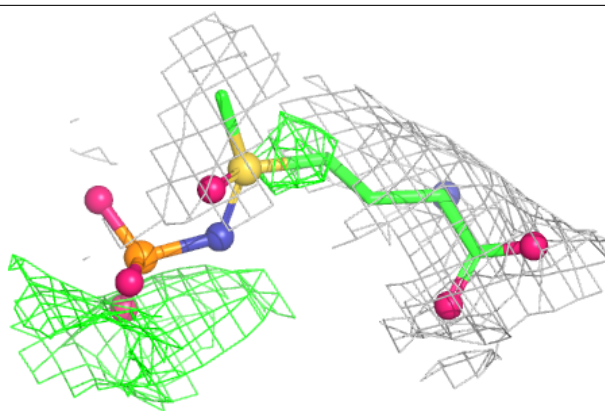
**Electron density around P3S J 502:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

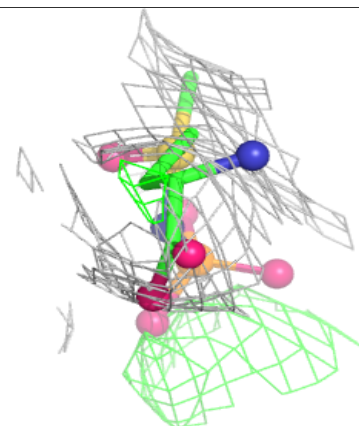
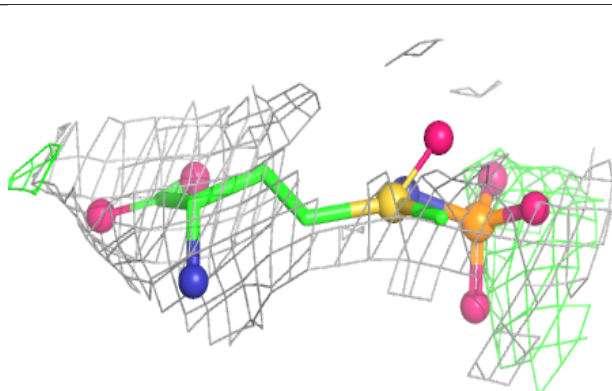
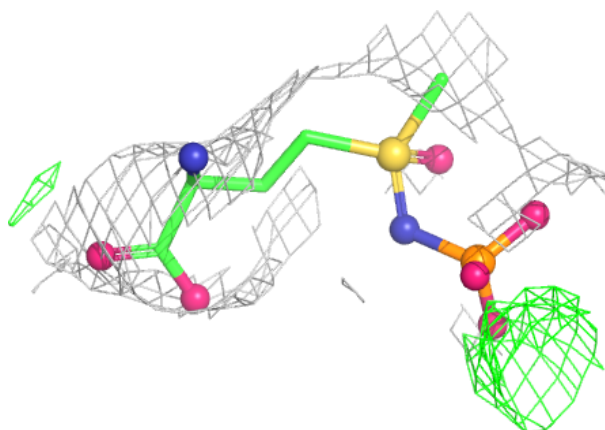


**Electron density around P3S M 502:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around P3S O 502:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.