



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:07 AM UTC

PDB ID : 7LMW / pdb_00007lmw
Title : Receptor for Advanced Glycation End Products VC1 domain in complex with
3-(3-((4-(4-carboxyphenoxy)benzyl)oxy)phenyl)-1H-indole-2-carboxylic acid
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Deposited on : 2021-02-06
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure 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/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>.

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)
Xtriage (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

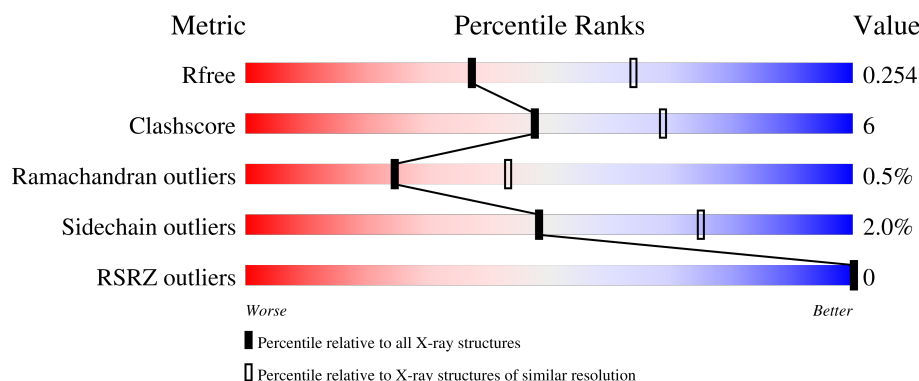
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 ≥ 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	212	
1	B	212	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	Y6P	B	503	-	X	-	-
2	Y6P	B	504	-	X	-	-
3	ACT	B	507	-	-	X	-
3	ACT	B	508	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3136 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.

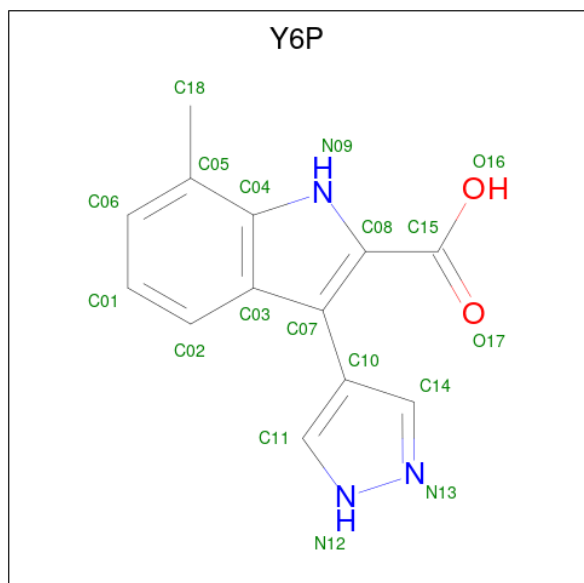
- Molecule 1 is a protein called Advanced glycosylation end product-specific receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	0
			1485	941	262	276	6			
1	B	208	Total	C	N	O	S	0	0	0
			1482	939	259	278	6			

There are 6 discrepancies between the modelled and reference sequences:

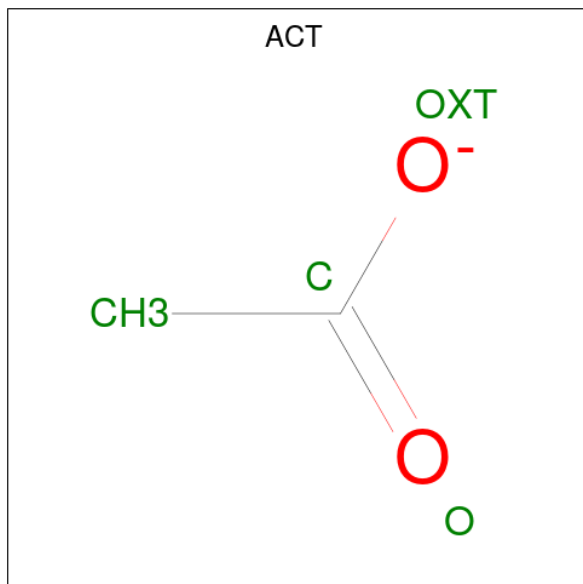
Chain	Residue	Modelled	Actual	Comment	Reference
A	20	GLY	-	expression tag	UNP Q15109
A	21	ALA	-	expression tag	UNP Q15109
A	22	MET	-	expression tag	UNP Q15109
B	20	GLY	-	expression tag	UNP Q15109
B	21	ALA	-	expression tag	UNP Q15109
B	22	MET	-	expression tag	UNP Q15109

- Molecule 2 is 7-methyl-3-(1 {H}-pyrazol-4-yl)-1 {H}-indole-2-carboxylic acid (CCD ID: Y6P) (formula: C₁₃H₁₁N₃O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			18	13	3	2		
2	A	1	Total	C	N	O	0	0
			18	13	3	2		
2	B	1	Total	C	N	O	0	0
			18	13	3	2		
2	B	1	Total	C	N	O	0	0
			18	13	3	2		
2	B	1	Total	C	N	O	0	0
			18	13	3	2		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2^-$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl^-).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Cl 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	20	Total 20	O 20	0	0
5	B	20	Total 20	O 20	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: Advanced glycosylation end product-specific receptor

Chain A:  87% 9% ..



- Molecule 1: Advanced glycosylation end product-specific receptor

Chain B:  86% 12% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α , β , γ	101.89Å 101.89Å 102.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	33.41 – 2.50 33.41 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (33.41-2.50) 96.7 (33.41-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.200 , 0.256 0.202 , 0.254	Depositor DCC
R_{free} test set	1084 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	38.4	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 21.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.479 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3136	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, ACT, Y6P

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	0.57	1/1525 (0.1%)	0.82	3/2092 (0.1%)
1	B	0.51	0/1521	0.68	0/2087
All	All	0.54	1/3046 (0.0%)	0.75	3/4179 (0.1%)

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	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	45	PRO	CA-C	5.72	1.55	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	TRP	N-CA-CB	12.79	132.10	110.49
1	A	230	TRP	CB-CA-C	-8.91	92.69	110.42
1	A	230	TRP	CA-CB-CG	8.61	129.96	113.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	229	VAL	Peptide

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Mol	Chain	Res	Type	Group
1	A	230	TRP	Peptide,Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1485	0	1395	11	1
1	B	1482	0	1391	21	1
2	A	36	0	0	0	0
2	B	72	0	0	2	0
3	A	8	0	6	1	0
3	B	12	0	9	12	0
4	B	1	0	0	0	0
5	A	20	0	0	0	0
5	B	20	0	0	0	0
All	All	3136	0	2801	33	1

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

All (33) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:ALA:H	3:B:508:ACT:H2	1.46	0.79
1:A:77:ARG:NH2	2:B:501:Y6P:O16	2.18	0.75
1:A:145:VAL:HG22	1:A:189:GLN:HG3	1.74	0.70
1:B:112:ASN:HD21	3:B:508:ACT:H3	1.61	0.64
1:B:145:VAL:HG22	1:B:189:GLN:HG3	1.79	0.64
1:B:21:ALA:H	3:B:508:ACT:CH3	2.12	0.60
1:B:21:ALA:N	3:B:508:ACT:H2	2.18	0.58
3:B:507:ACT:OXT	3:B:508:ACT:H1	2.04	0.58
1:B:98:ARG:HH21	3:B:508:ACT:H1	1.69	0.57
1:B:21:ALA:HB3	3:B:508:ACT:H2	1.86	0.57
1:B:98:ARG:HH21	3:B:508:ACT:CH3	2.19	0.56
1:B:112:ASN:HD21	3:B:508:ACT:CH3	2.19	0.54
1:B:175:GLU:HG2	1:B:176:GLN:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:LYS:HZ1	2:B:504:Y6P:C15	2.24	0.51
1:A:212:PRO:HG2	1:A:217:HIS:HB2	1.93	0.50
1:B:94:GLU:HG2	1:B:117:VAL:HG13	1.93	0.49
1:B:112:ASN:ND2	3:B:508:ACT:H3	2.28	0.48
1:A:133:LEU:O	1:A:229:VAL:HA	2.13	0.48
1:A:23:ALA:HB2	3:A:404:ACT:H1	1.97	0.47
1:B:208:CYS:O	1:B:222:THR:HG23	2.15	0.47
1:A:146:SER:HB2	1:A:155:LEU:HD21	1.98	0.45
1:A:132:GLU:HG3	1:A:228:ARG:HG2	1.97	0.45
1:B:98:ARG:HH22	3:B:506:ACT:C	2.31	0.44
1:B:29:ARG:HB3	1:B:32:GLU:HG3	1.98	0.44
1:B:96:ILE:HD13	3:B:507:ACT:OXT	2.18	0.44
1:A:132:GLU:OE1	1:A:228:ARG:NH2	2.52	0.42
1:B:28:ALA:O	1:B:117:VAL:HA	2.18	0.42
1:B:35:VAL:HG22	1:B:85:PHE:HD1	1.85	0.42
1:B:133:LEU:HB2	1:B:229:VAL:HG22	2.02	0.42
1:A:28:ALA:O	1:A:117:VAL:HA	2.20	0.41
1:A:94:GLU:HG3	1:A:116:ARG:HA	2.02	0.40
1:A:103:ASN:HD22	1:A:103:ASN:N	2.18	0.40
1:B:127:VAL:O	1:B:128:ASP:C	2.65	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:GLU:OE2	1:B:25:ASN:ND2[5_554]	1.87	0.33

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	204/212 (96%)	201 (98%)	2 (1%)	1 (0%)	24 43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	204/212 (96%)	201 (98%)	2 (1%)	1 (0%)	24	43
All	All	408/424 (96%)	402 (98%)	4 (1%)	2 (0%)	24	43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	168	GLU
1	B	168	GLU

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 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	147/176 (84%)	143 (97%)	4 (3%)	39	67
1	B	147/176 (84%)	145 (99%)	2 (1%)	59	81
All	All	294/352 (84%)	288 (98%)	6 (2%)	48	75

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	GLU
1	A	131	SER
1	A	179	ARG
1	A	230	TRP
1	B	156	SER
1	B	182	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	B	100	GLN
1	B	112	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 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$
2	Y6P	B	502	-	20,20,20	4.73	9 (45%)	26,29,29	1.23	3 (11%)
3	ACT	A	403	-	3,3,3	1.83	1 (33%)	3,3,3	1.32	0
2	Y6P	A	401	-	20,20,20	4.65	8 (40%)	26,29,29	1.40	4 (15%)
2	Y6P	A	402	-	20,20,20	4.83	8 (40%)	26,29,29	1.42	2 (7%)
2	Y6P	B	504	-	20,20,20	5.20	10 (50%)	26,29,29	2.06	8 (30%)
2	Y6P	B	503	-	20,20,20	5.00	9 (45%)	26,29,29	2.10	7 (26%)
3	ACT	B	507	-	3,3,3	1.71	1 (33%)	3,3,3	1.45	1 (33%)
3	ACT	A	404	-	3,3,3	1.55	1 (33%)	3,3,3	1.64	1 (33%)
2	Y6P	B	501	-	20,20,20	4.72	9 (45%)	26,29,29	1.45	4 (15%)
3	ACT	B	508	-	3,3,3	0.81	0	3,3,3	1.63	1 (33%)
3	ACT	B	506	-	3,3,3	1.73	1 (33%)	3,3,3	1.51	0

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	Y6P	B	502	-	-	5/8/8/8	0/3/3/3
2	Y6P	A	401	-	-	4/8/8/8	0/3/3/3
2	Y6P	A	402	-	-	4/8/8/8	0/3/3/3
2	Y6P	B	504	-	-	8/8/8/8	0/3/3/3
2	Y6P	B	503	-	-	8/8/8/8	0/3/3/3
2	Y6P	B	501	-	-	4/8/8/8	0/3/3/3

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	503	Y6P	C04-C05	13.45	1.59	1.40
2	B	501	Y6P	C04-C05	12.70	1.58	1.40
2	B	504	Y6P	C04-C05	12.58	1.58	1.40
2	B	504	Y6P	C02-C03	12.35	1.58	1.39
2	B	503	Y6P	C02-C03	12.05	1.58	1.39
2	A	402	Y6P	C04-C05	12.05	1.57	1.40
2	B	502	Y6P	C04-C05	11.68	1.57	1.40
2	A	401	Y6P	C04-C05	11.31	1.56	1.40
2	B	501	Y6P	C02-C03	11.13	1.56	1.39
2	B	502	Y6P	C02-C03	11.11	1.56	1.39
2	A	401	Y6P	C02-C03	11.02	1.56	1.39
2	A	402	Y6P	C02-C03	11.00	1.56	1.39
2	B	504	Y6P	C01-C02	8.04	1.52	1.38
2	A	402	Y6P	C01-C02	7.63	1.51	1.38
2	B	502	Y6P	C01-C02	7.51	1.51	1.38
2	B	503	Y6P	C01-C02	7.25	1.51	1.38
2	A	401	Y6P	C01-C02	7.19	1.51	1.38
2	B	501	Y6P	C01-C02	6.93	1.50	1.38
2	B	504	Y6P	C06-C05	6.68	1.53	1.39
2	B	504	Y6P	C01-C06	6.51	1.50	1.38
2	A	402	Y6P	C01-C06	6.45	1.49	1.38
2	A	401	Y6P	C01-C06	6.34	1.49	1.38
2	B	502	Y6P	C01-C06	6.29	1.49	1.38
2	A	402	Y6P	C06-C05	5.92	1.51	1.39
2	B	503	Y6P	C06-C05	5.69	1.51	1.39
2	B	504	Y6P	C08-C15	5.63	1.56	1.48
2	B	501	Y6P	C01-C06	5.60	1.48	1.38
2	B	502	Y6P	C06-C05	5.51	1.50	1.39
2	B	503	Y6P	C01-C06	5.44	1.48	1.38
2	A	401	Y6P	C06-C05	5.34	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	Y6P	C06-C05	5.15	1.50	1.39
2	B	502	Y6P	C07-C10	4.73	1.54	1.44
2	A	402	Y6P	C07-C10	4.70	1.54	1.44
2	B	501	Y6P	C03-C07	-4.41	1.36	1.46
2	A	401	Y6P	C07-C10	4.39	1.53	1.44
2	B	504	Y6P	C07-C10	4.17	1.53	1.44
2	A	401	Y6P	C03-C07	-4.07	1.36	1.46
2	B	502	Y6P	C03-C07	-4.05	1.37	1.46
2	A	402	Y6P	C03-C07	-3.87	1.37	1.46
2	B	503	Y6P	C07-C10	3.81	1.52	1.44
2	B	503	Y6P	C08-C15	3.64	1.53	1.48
2	A	402	Y6P	C08-C15	3.64	1.53	1.48
2	B	503	Y6P	C03-C07	-3.47	1.38	1.46
2	B	501	Y6P	C07-C10	3.46	1.51	1.44
2	B	504	Y6P	C03-C07	-3.27	1.38	1.46
2	B	503	Y6P	C03-C04	-2.81	1.37	1.41
3	B	506	ACT	CH3-C	2.73	1.59	1.49
3	A	403	ACT	CH3-C	2.69	1.59	1.49
2	A	401	Y6P	N12-N13	2.54	1.41	1.35
2	B	502	Y6P	C08-C15	2.42	1.52	1.48
2	B	502	Y6P	N12-N13	2.39	1.41	1.35
2	B	501	Y6P	C08-C15	2.32	1.51	1.48
3	A	404	ACT	CH3-C	2.30	1.58	1.49
2	B	501	Y6P	N12-N13	2.19	1.40	1.35
3	B	507	ACT	CH3-C	2.08	1.57	1.49
2	B	504	Y6P	C03-C04	-2.03	1.39	1.41
2	B	504	Y6P	N12-N13	2.02	1.40	1.35

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	503	Y6P	C07-C08-N09	-5.20	105.22	109.57
2	B	504	Y6P	C07-C08-N09	-4.81	105.54	109.57
2	B	504	Y6P	C18-C05-C04	-4.34	116.14	121.42
2	B	504	Y6P	O16-C15-C08	4.10	123.23	116.73
2	B	503	Y6P	C03-C07-C08	3.62	109.20	106.49
2	B	504	Y6P	C03-C07-C08	3.59	109.17	106.49
2	B	503	Y6P	C03-C04-C05	-3.48	119.59	123.28
2	B	501	Y6P	C04-C03-C07	3.34	109.14	106.87
2	A	402	Y6P	C15-C08-N09	3.30	125.32	121.22
2	B	503	Y6P	C11-C10-C14	3.23	109.18	104.28
2	A	401	Y6P	C10-C14-N13	-3.22	106.59	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	503	Y6P	C06-C05-C04	3.15	122.14	117.76
2	A	401	Y6P	C11-C10-C14	2.93	108.72	104.28
2	B	501	Y6P	C03-C07-C10	-2.88	118.56	125.02
2	B	504	Y6P	O16-C15-O17	-2.77	117.30	123.90
2	B	503	Y6P	C05-C04-N09	2.77	133.72	128.06
2	B	501	Y6P	C11-C10-C14	2.56	108.15	104.28
2	B	504	Y6P	C11-C10-C14	2.53	108.12	104.28
2	B	502	Y6P	C04-C03-C07	2.41	108.51	106.87
2	B	504	Y6P	C15-C08-N09	2.41	124.22	121.22
2	B	501	Y6P	C03-C04-C05	-2.32	120.82	123.28
2	B	503	Y6P	C10-C14-N13	-2.30	108.01	111.56
2	A	401	Y6P	C18-C05-C04	-2.24	118.70	121.42
2	B	502	Y6P	C11-C10-C14	2.24	107.67	104.28
3	B	507	ACT	OXT-C-O	2.14	129.97	122.03
3	B	508	ACT	O-C-CH3	-2.14	113.77	122.53
2	A	402	Y6P	C07-C08-N09	-2.13	107.79	109.57
2	B	504	Y6P	C01-C06-C05	-2.09	117.85	121.14
2	B	502	Y6P	C15-C08-N09	2.09	123.82	121.22
3	A	404	ACT	O-C-CH3	-2.05	114.11	122.53
2	A	401	Y6P	C11-N12-N13	-2.04	107.05	111.25

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	Y6P	C07-C08-C15-O16
2	A	401	Y6P	N09-C08-C15-O16
2	A	401	Y6P	C07-C08-C15-O17
2	A	401	Y6P	N09-C08-C15-O17
2	B	501	Y6P	C07-C08-C15-O16
2	B	501	Y6P	N09-C08-C15-O16
2	B	501	Y6P	C07-C08-C15-O17
2	B	501	Y6P	N09-C08-C15-O17
2	B	502	Y6P	C07-C08-C15-O16
2	B	502	Y6P	N09-C08-C15-O16
2	B	502	Y6P	C07-C08-C15-O17
2	B	502	Y6P	N09-C08-C15-O17
2	B	503	Y6P	C03-C07-C10-C11
2	B	503	Y6P	C08-C07-C10-C14
2	B	503	Y6P	C07-C08-C15-O16
2	B	503	Y6P	N09-C08-C15-O16
2	B	503	Y6P	C07-C08-C15-O17

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Mol	Chain	Res	Type	Atoms
2	B	503	Y6P	N09-C08-C15-O17
2	B	504	Y6P	C03-C07-C10-C11
2	B	504	Y6P	C08-C07-C10-C11
2	B	504	Y6P	C08-C07-C10-C14
2	B	504	Y6P	C07-C08-C15-O16
2	B	504	Y6P	N09-C08-C15-O16
2	B	504	Y6P	C07-C08-C15-O17
2	B	504	Y6P	N09-C08-C15-O17
2	A	402	Y6P	N09-C08-C15-O16
2	A	402	Y6P	N09-C08-C15-O17
2	A	402	Y6P	C07-C08-C15-O16
2	A	402	Y6P	C07-C08-C15-O17
2	B	502	Y6P	C03-C07-C10-C11
2	B	503	Y6P	C08-C07-C10-C11
2	B	503	Y6P	C03-C07-C10-C14
2	B	504	Y6P	C03-C07-C10-C14

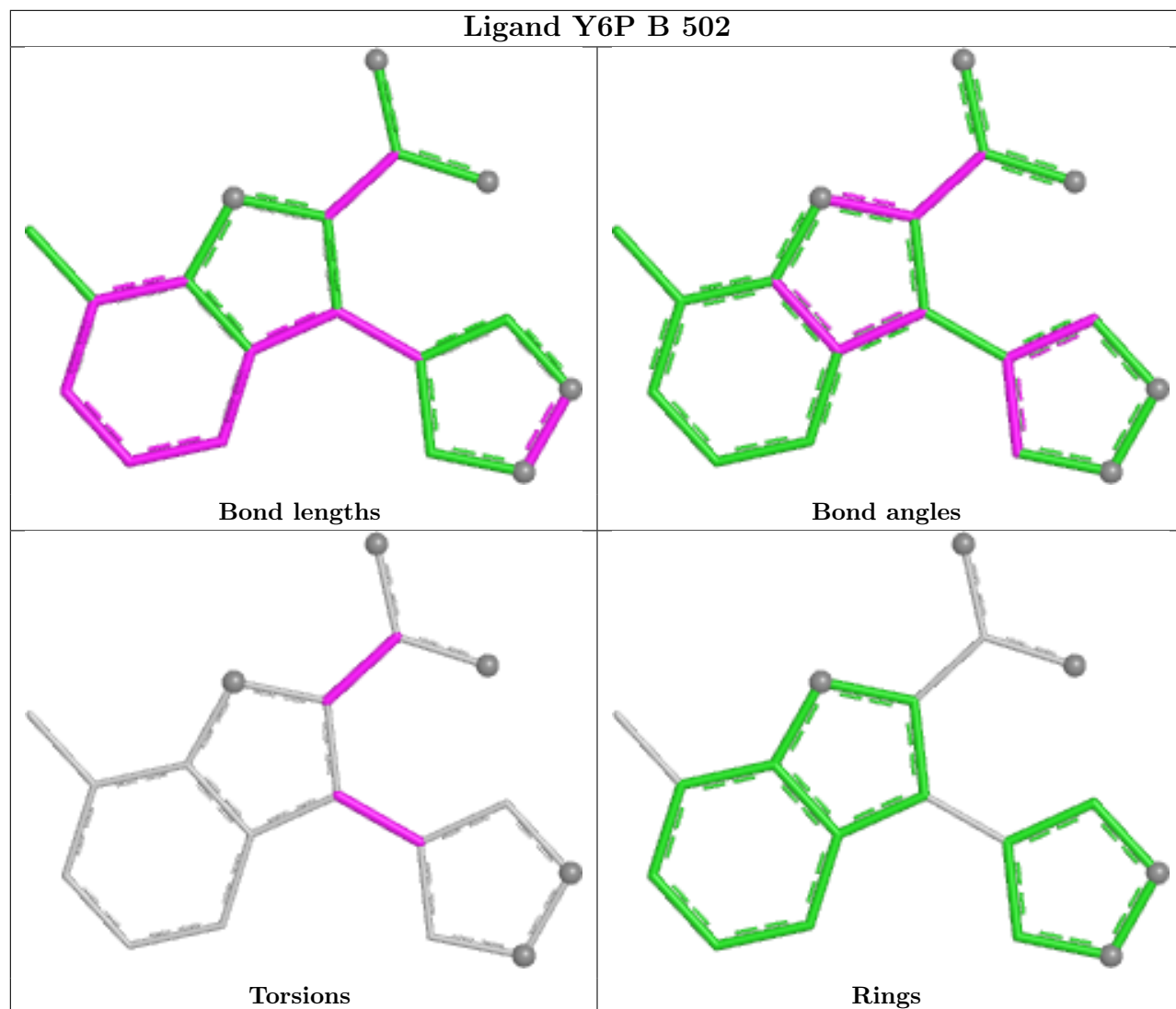
There are no ring outliers.

6 monomers are involved in 15 short contacts:

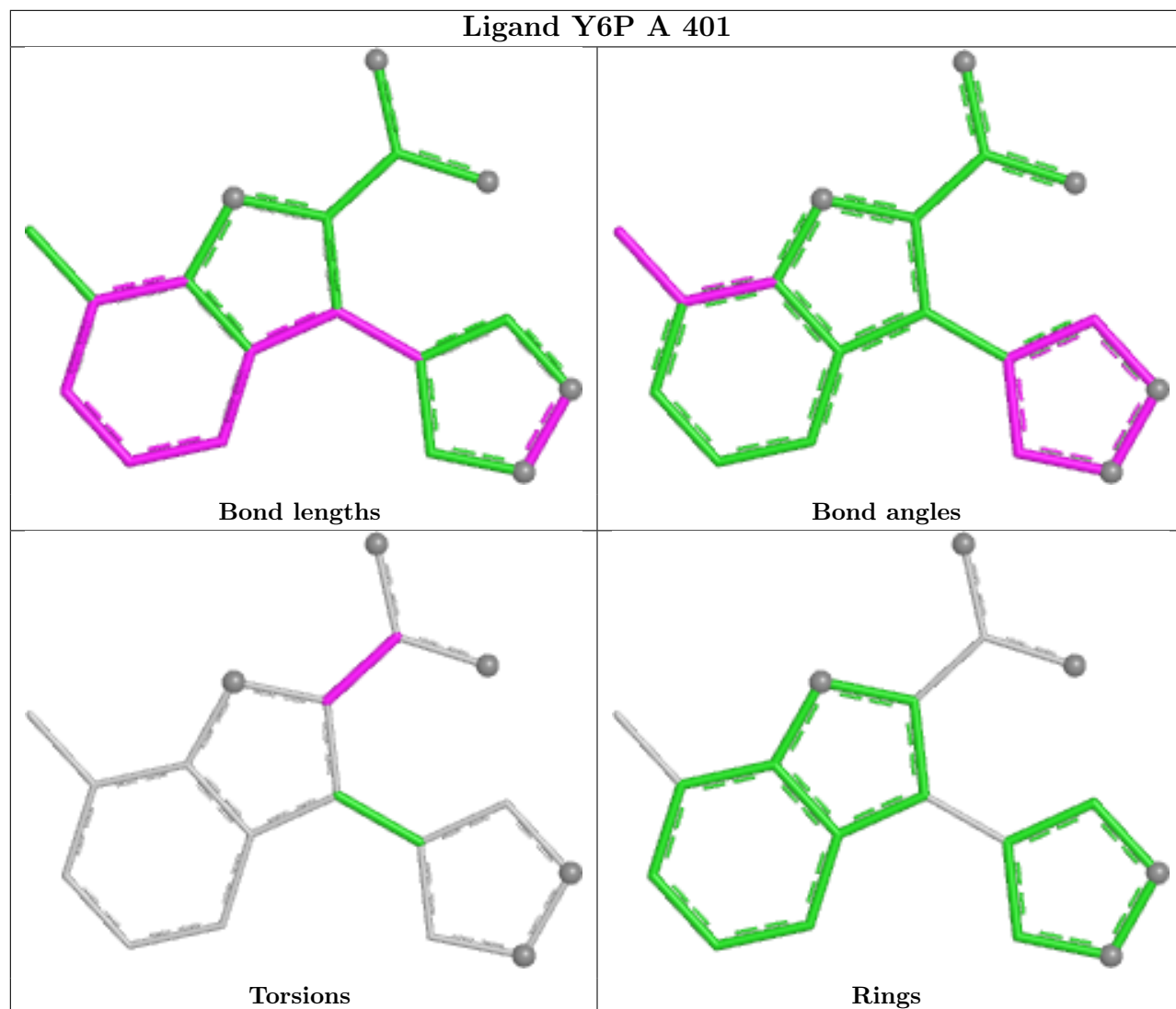
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	504	Y6P	1	0
3	B	507	ACT	2	0
3	A	404	ACT	1	0
2	B	501	Y6P	1	0
3	B	508	ACT	10	0
3	B	506	ACT	1	0

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.

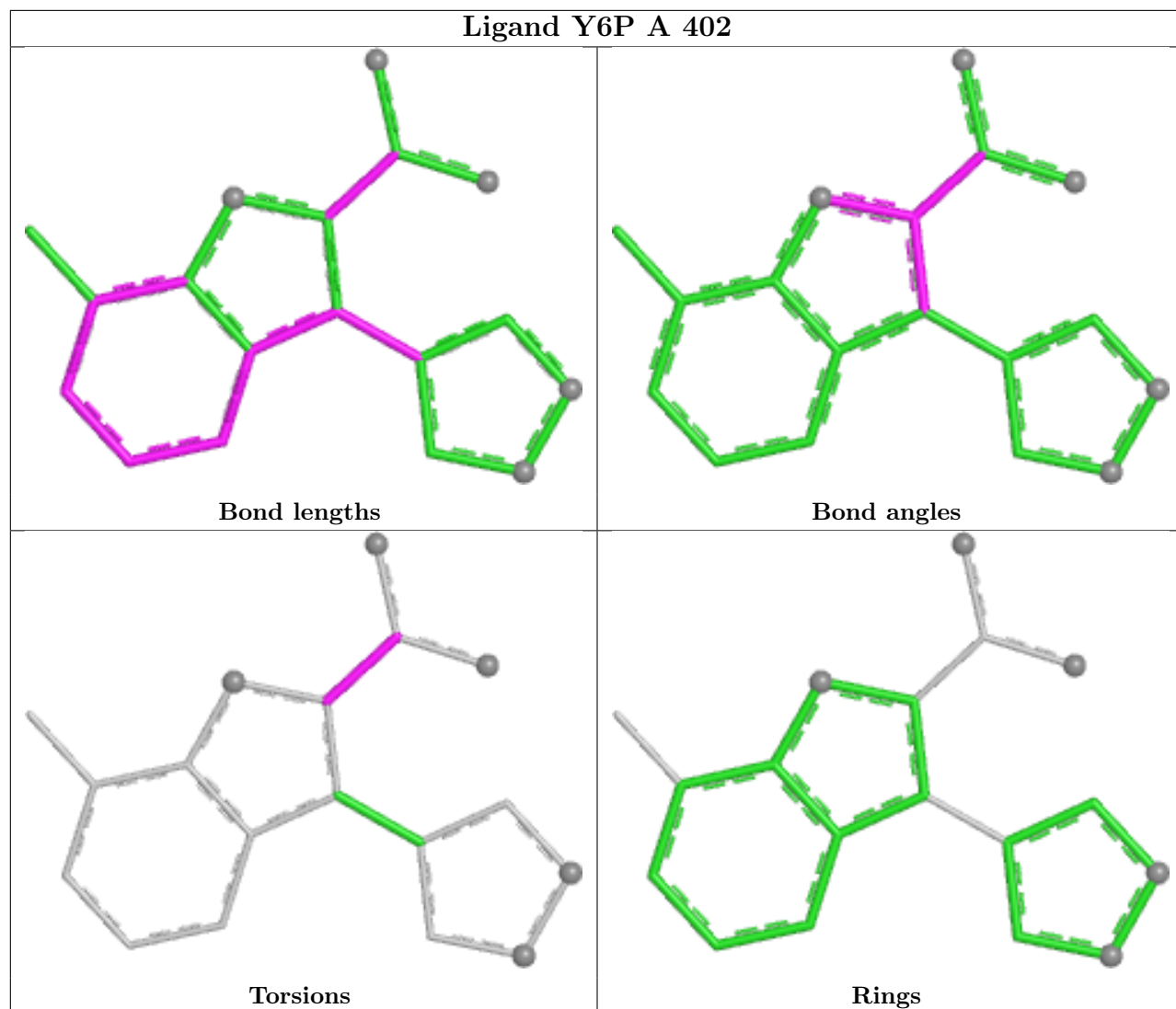
Ligand Y6P B 502



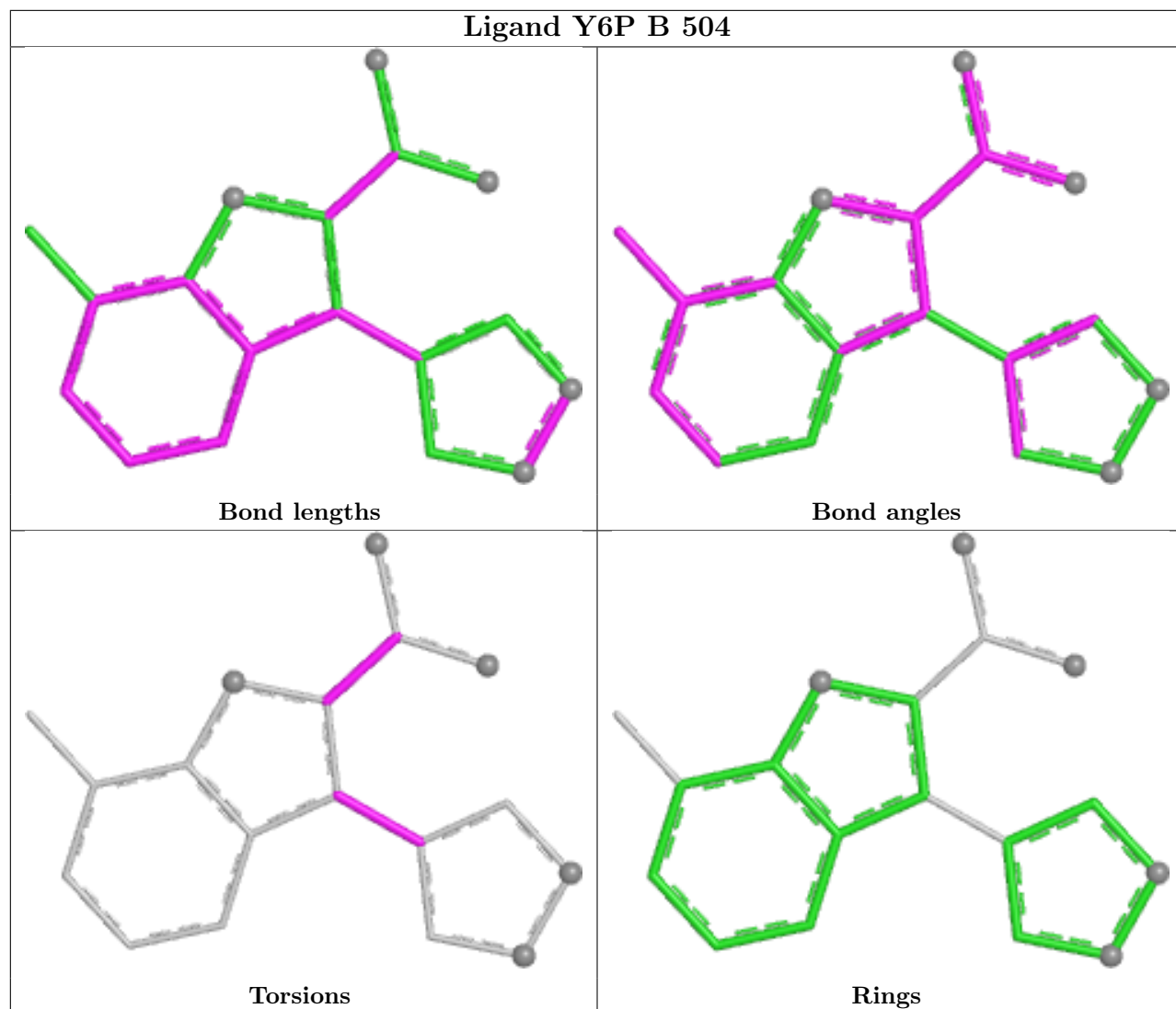
Ligand Y6P A 401



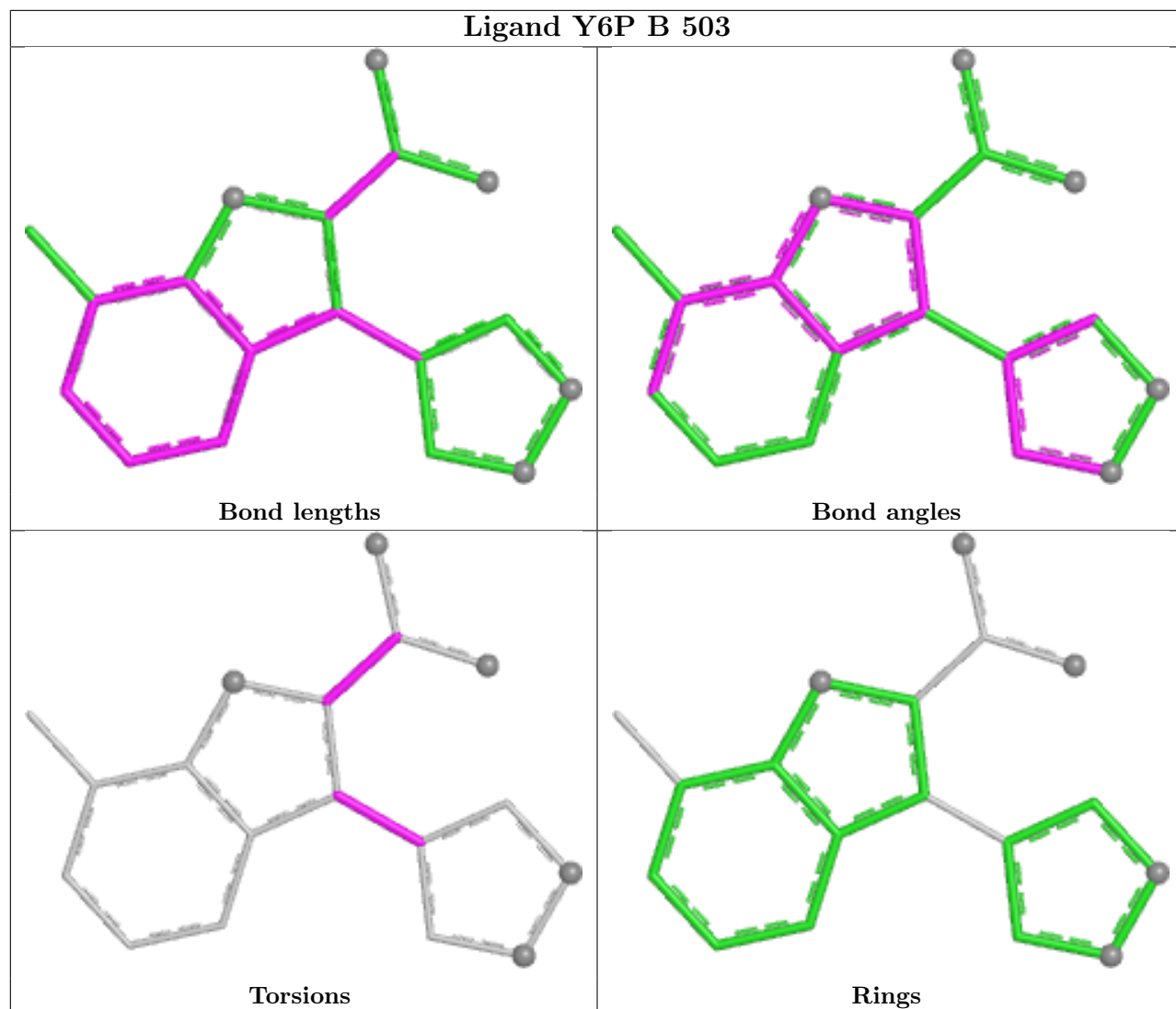
Ligand Y6P A 402

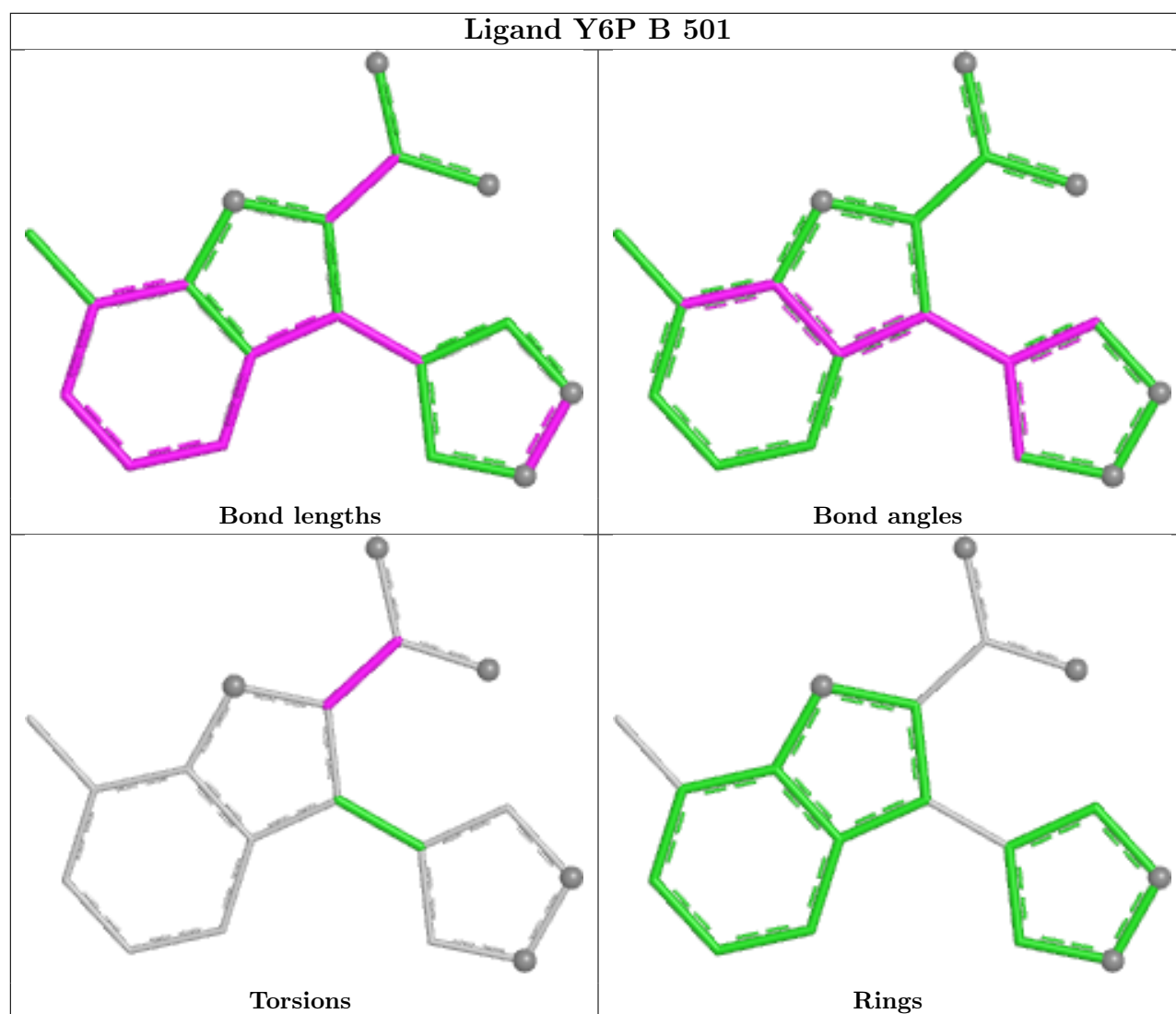


Ligand Y6P B 504



Ligand Y6P B 503





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, 95th 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 ²)	Q<0.9
1	A	208/212 (98%)	-1.36	0 100 100	24, 42, 86, 126	0
1	B	208/212 (98%)	-1.36	0 100 100	24, 44, 90, 117	0
All	All	416/424 (98%)	-1.36	0 100 100	24, 44, 87, 126	0

There are no RSRZ outliers to report.

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 [i](#)

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, 95th 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 ²)	Q<0.9
2	Y6P	A	402	18/18	0.98	0.06	50,59,71,72	18
2	Y6P	B	501	18/18	0.98	0.06	42,61,81,87	0
2	Y6P	B	503	18/18	0.98	0.06	43,68,81,82	0
2	Y6P	B	504	18/18	0.98	0.06	39,59,69,76	18
3	ACT	B	507	4/4	0.98	0.12	125,134,139,142	0
2	Y6P	B	502	18/18	0.99	0.04	30,43,57,66	18
3	ACT	A	404	4/4	0.99	0.09	31,42,42,49	0

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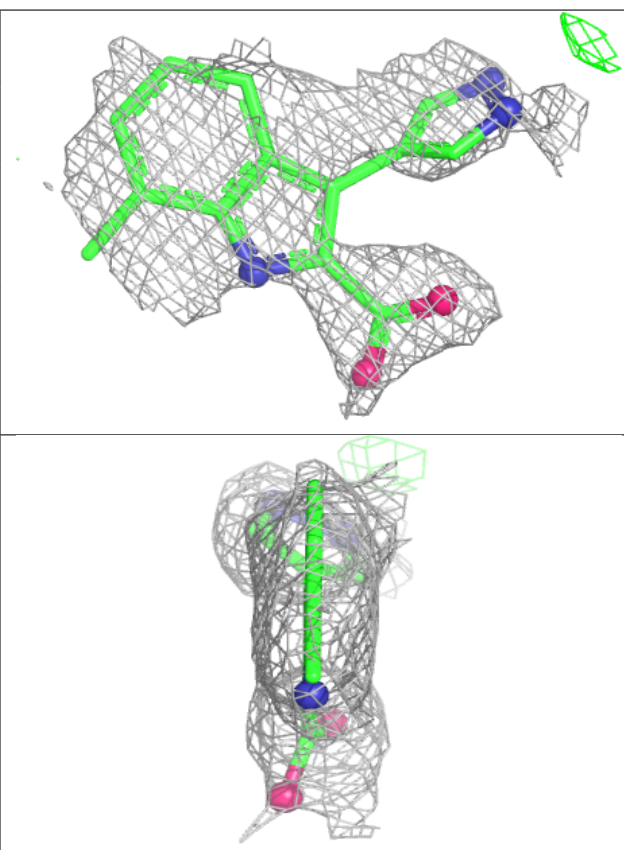
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ACT	B	506	4/4	0.99	0.04	44,50,52,55	0
2	Y6P	A	401	18/18	0.99	0.04	28,45,59,68	18
3	ACT	A	403	4/4	1.00	0.03	38,40,53,54	0
3	ACT	B	508	4/4	1.00	0.05	56,59,73,73	0
4	CL	B	505	1/1	1.00	0.02	50,50,50,50	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.

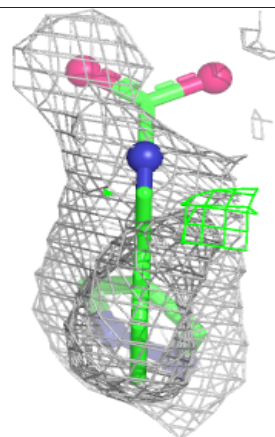
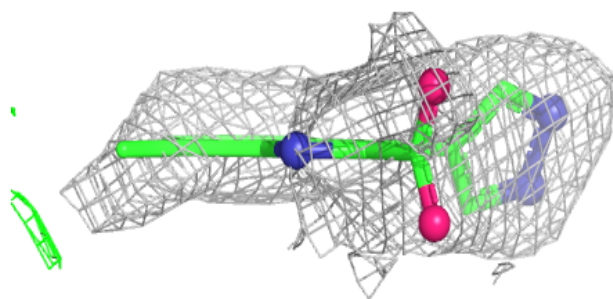
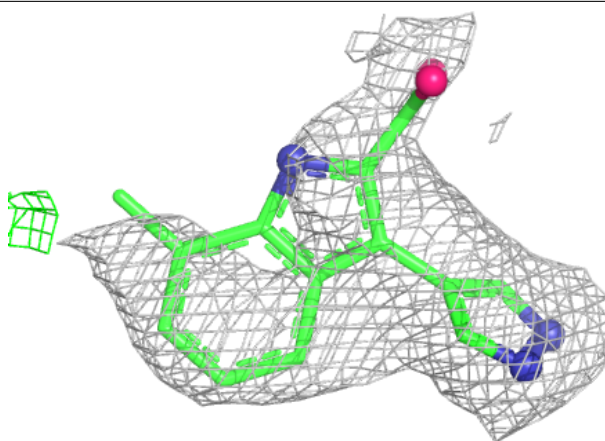
Electron density around Y6P A 402:

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



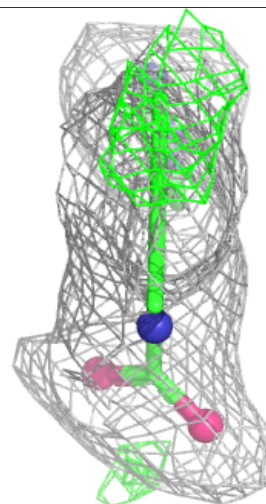
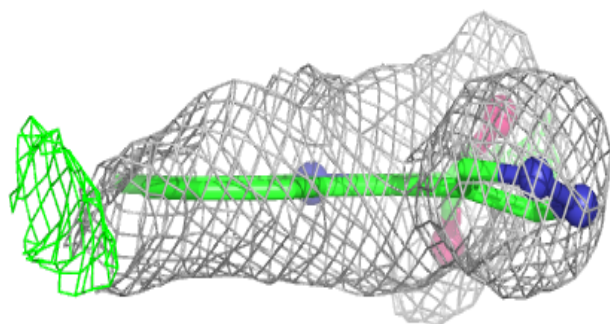
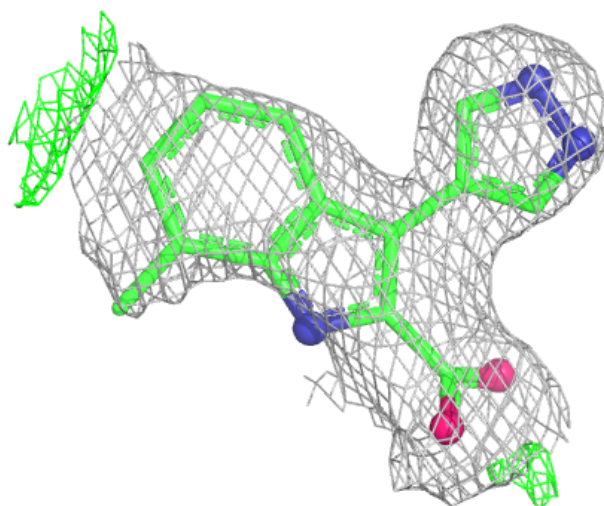
Electron density around Y6P B 501:

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



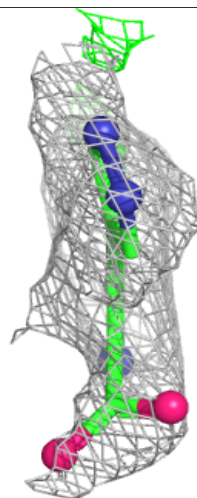
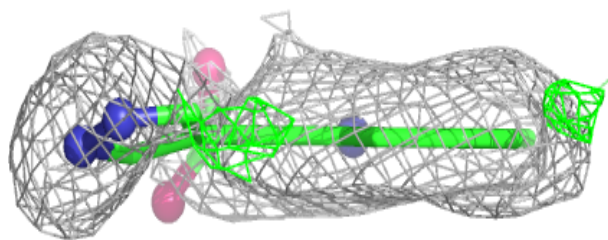
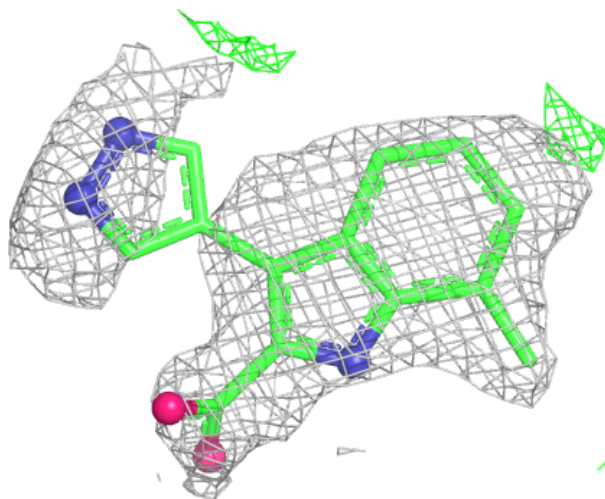
Electron density around Y6P B 503:

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



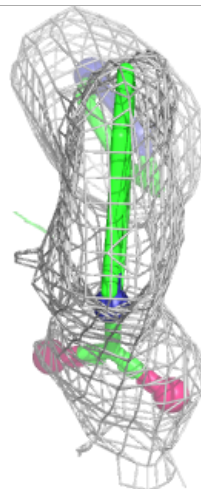
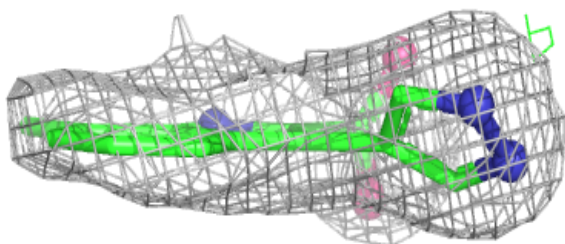
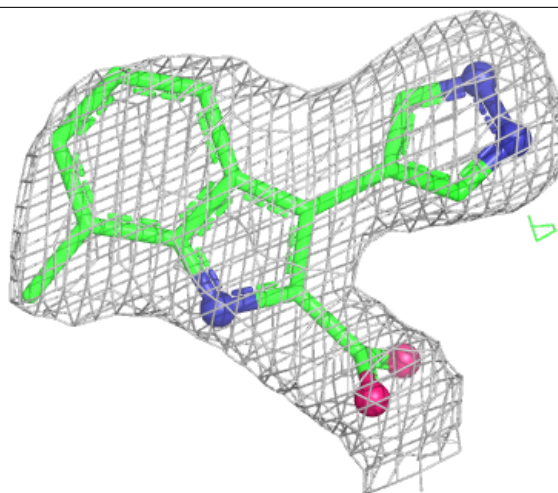
Electron density around Y6P B 504:

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



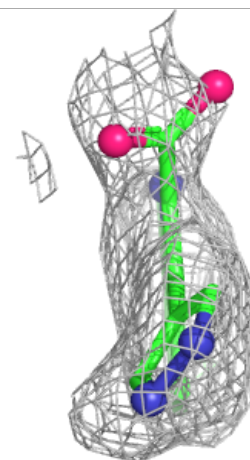
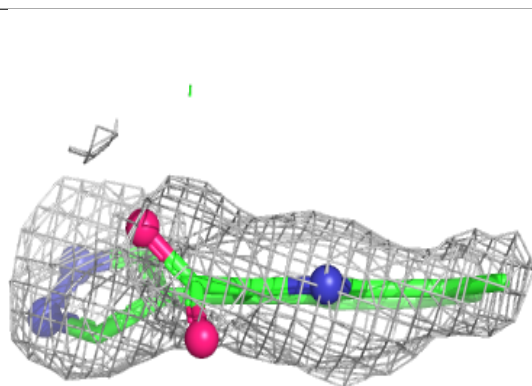
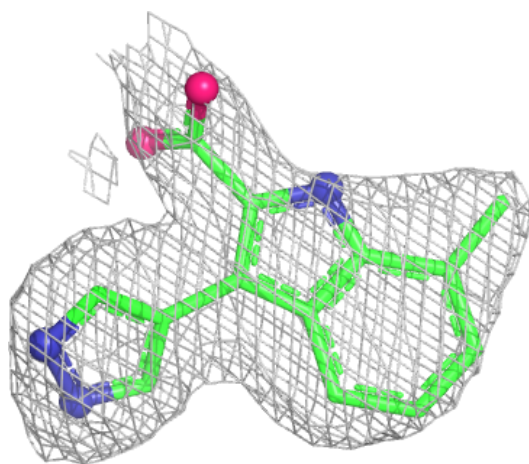
Electron density around Y6P B 502:

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



Electron density around Y6P A 401:

$2mF_o-DF_c$ (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.