



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 21, 2026 – 06:08 PM EDT

PDB ID : 9MDT / pdb_00009mdt
Title : Crystal Structure Pyrophosphate-fructose 6-phosphate 1-phosphotransferase 1 (Pfk1) from Trichomonas vaginalis (AMP/Pyrophosphate complex)
Authors : Seattle Structural Genomics Center for Infectious Disease; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2024-12-05
Resolution : 2.16 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

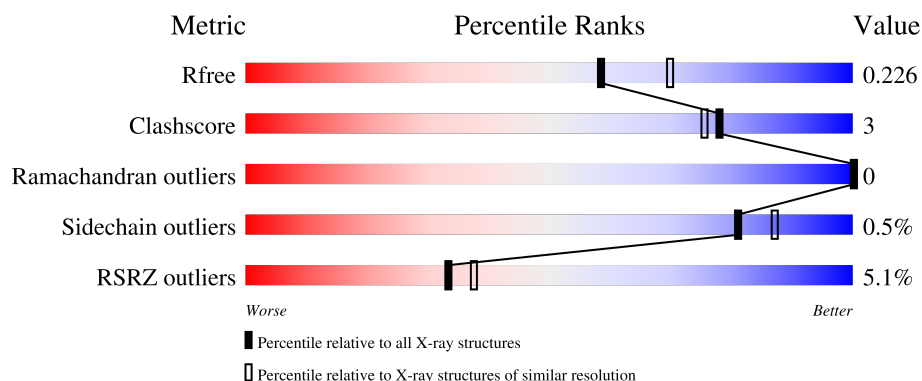
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.16 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	434	8% 87% 9% .
1	B	434	3% 90% 8% .
1	C	434	4% 91% 6% .
1	D	434	5% 91% 5% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13216 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 Pyrophosphate--fructose 6-phosphate 1-phosphotransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	0	0
			3191	2028	556	591	16			
1	B	423	Total	C	N	O	S	0	0	0
			3244	2059	565	603	17			
1	C	423	Total	C	N	O	S	0	0	0
			3244	2060	566	601	17			
1	D	418	Total	C	N	O	S	0	0	0
			3189	2024	554	594	17			

There are 32 discrepancies between the modelled and reference sequences:

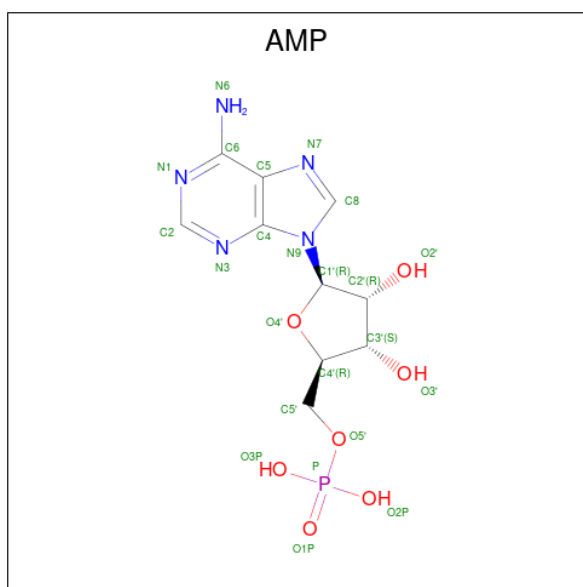
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP O61068
A	-6	ALA	-	expression tag	UNP O61068
A	-5	HIS	-	expression tag	UNP O61068
A	-4	HIS	-	expression tag	UNP O61068
A	-3	HIS	-	expression tag	UNP O61068
A	-2	HIS	-	expression tag	UNP O61068
A	-1	HIS	-	expression tag	UNP O61068
A	0	HIS	-	expression tag	UNP O61068
B	-7	MET	-	initiating methionine	UNP O61068
B	-6	ALA	-	expression tag	UNP O61068
B	-5	HIS	-	expression tag	UNP O61068
B	-4	HIS	-	expression tag	UNP O61068
B	-3	HIS	-	expression tag	UNP O61068
B	-2	HIS	-	expression tag	UNP O61068
B	-1	HIS	-	expression tag	UNP O61068
B	0	HIS	-	expression tag	UNP O61068
C	-7	MET	-	initiating methionine	UNP O61068
C	-6	ALA	-	expression tag	UNP O61068
C	-5	HIS	-	expression tag	UNP O61068
C	-4	HIS	-	expression tag	UNP O61068
C	-3	HIS	-	expression tag	UNP O61068

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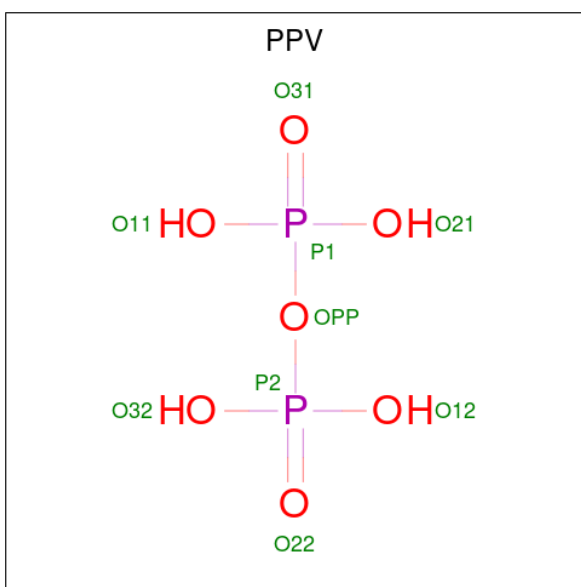
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	HIS	-	expression tag	UNP O61068
C	-1	HIS	-	expression tag	UNP O61068
C	0	HIS	-	expression tag	UNP O61068
D	-7	MET	-	initiating methionine	UNP O61068
D	-6	ALA	-	expression tag	UNP O61068
D	-5	HIS	-	expression tag	UNP O61068
D	-4	HIS	-	expression tag	UNP O61068
D	-3	HIS	-	expression tag	UNP O61068
D	-2	HIS	-	expression tag	UNP O61068
D	-1	HIS	-	expression tag	UNP O61068
D	0	HIS	-	expression tag	UNP O61068

- Molecule 2 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$) (labeled as "Ligand of Interest" by depositor).



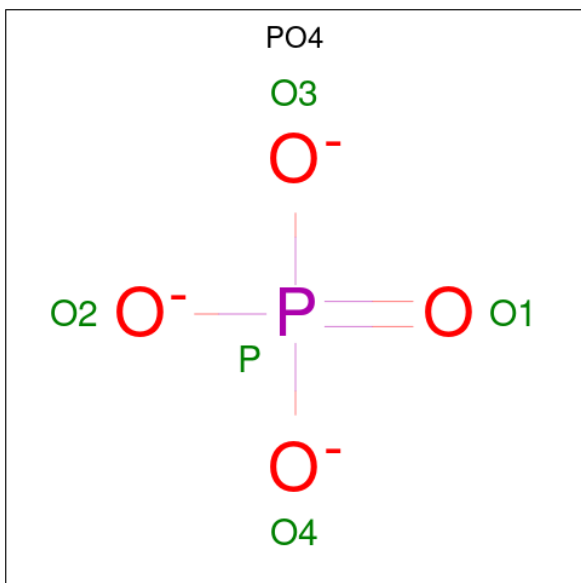
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 3 is PYROPHOSPHATE (CCD ID: PPV) (formula: $H_4O_7P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			9	7	2		
3	B	1	Total	O	P	0	0
			9	7	2		
3	C	1	Total	O	P	0	0
			9	7	2		
3	D	1	Total	O	P	0	0
			9	7	2		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 5 4 1	0	0
4	A	1	Total O P 5 4 1	0	0
4	B	1	Total O P 5 4 1	0	0
4	B	1	Total O P 5 4 1	0	0
4	C	1	Total O P 5 4 1	0	0
4	C	1	Total O P 5 4 1	0	0
4	D	1	Total O P 5 4 1	0	0
4	D	1	Total O P 5 4 1	0	0

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Cl 2 2	0	0
5	B	2	Total Cl 2 2	0	0
5	D	2	Total Cl 2 2	0	0

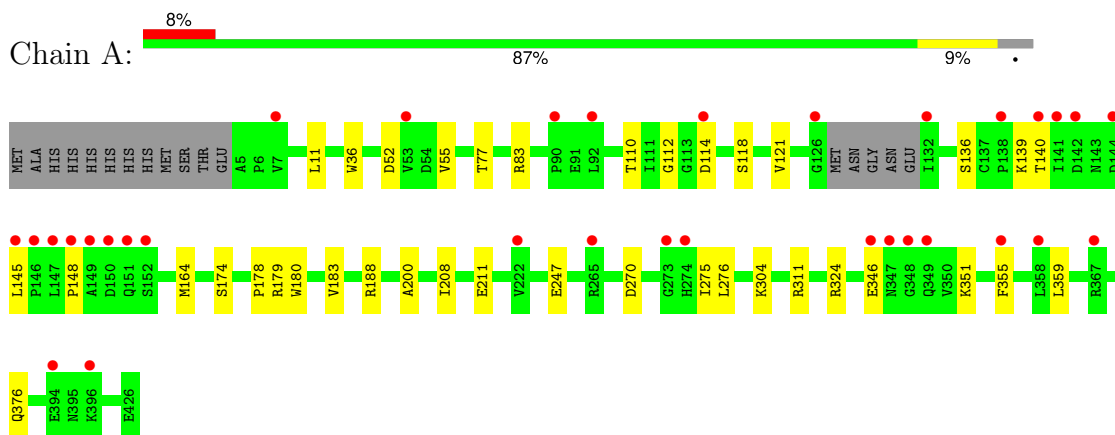
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	54	Total O 54 54	0	0
6	B	40	Total O 40 40	0	0
6	C	50	Total O 50 50	0	0
6	D	30	Total O 30 30	0	0

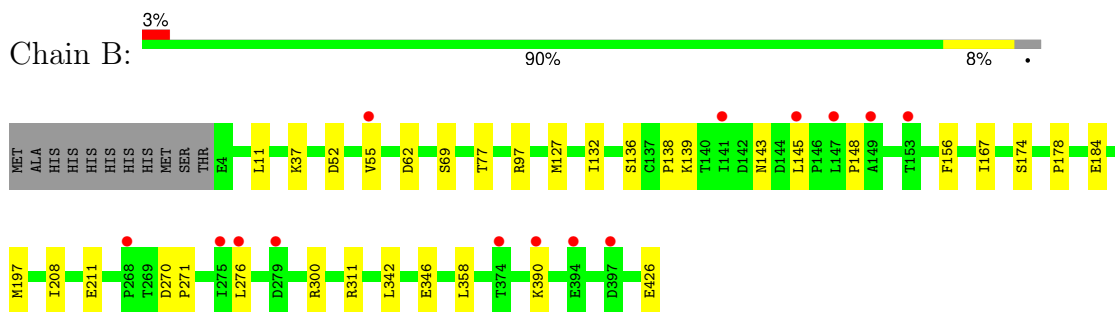
3 Residue-property plots [i](#)

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.

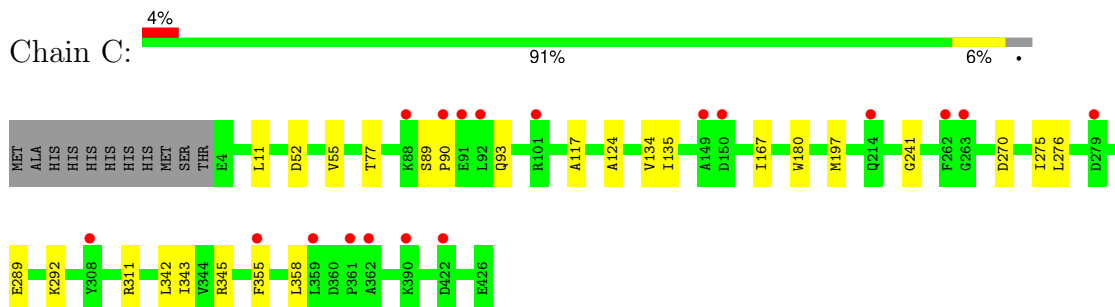
- Molecule 1: Pyrophosphate--fructose 6-phosphate 1-phosphotransferase 1



- Molecule 1: Pyrophosphate--fructose 6-phosphate 1-phosphotransferase 1



- Molecule 1: Pyrophosphate--fructose 6-phosphate 1-phosphotransferase 1



- Molecule 1: Pyrophosphate--fructose 6-phosphate 1-phosphotransferase 1

L276	MT
K292	ALA
R300	HIS
R311	HIS
L342	HIS
I343	HIS
F365	MT
L358	SR
D360	THR
P361	GLU
A362	A5
T363	L11
G364	D52
R365	V55
V366	D114
R367	D115
T368	A124
E426	V134
	P138
	K139
	T140
	I141
	L145
	P146
	L147
	A159
	I167
	S174
	P178
	M197
	I217
	K252
	Y259
	R265
	D270
	PRO
	HIS
	GLY
	THR

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	87.11Å 87.11Å 478.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.74 – 2.16 48.74 – 2.16	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.74-2.16) 100.0 (48.74-2.16)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.16Å)	Xtriage
Refinement program	PHENIX 2.0_5936	Depositor
R, R_{free}	0.191 , 0.226 0.197 , 0.226	Depositor DCC
R_{free} test set	4984 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	46.5	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13216	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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: AMP, PO4, CL, PPV

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	0.30	0/3250	0.46	0/4396
1	B	0.27	0/3304	0.43	0/4468
1	C	0.28	0/3304	0.45	0/4467
1	D	0.26	0/3245	0.43	0/4389
All	All	0.28	0/13103	0.44	0/17720

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	311	ARG	Sidechain
1	B	311	ARG	Sidechain
1	C	311	ARG	Sidechain
1	D	311	ARG	Sidechain

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	3191	0	3231	28	0
1	B	3244	0	3288	20	0
1	C	3244	0	3295	15	0
1	D	3189	0	3222	10	0
2	A	23	0	12	0	0
2	B	46	0	24	0	0
2	C	23	0	12	0	0
3	A	9	0	0	1	0
3	B	9	0	0	0	0
3	C	9	0	0	0	0
3	D	9	0	0	0	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
4	C	10	0	0	0	0
4	D	10	0	0	1	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	D	2	0	0	0	0
6	A	54	0	0	1	0
6	B	40	0	0	1	0
6	C	50	0	0	1	0
6	D	30	0	0	0	0
All	All	13216	0	13084	73	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 (73) 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:A:148:PRO:HG2	1:A:346:GLU:HG2	1.66	0.78
1:A:121:VAL:HG11	1:A:355:PHE:CG	2.23	0.74
1:A:121:VAL:HG11	1:A:355:PHE:CD2	2.23	0.73
1:C:124:ALA:HB2	1:C:134:VAL:HG21	1.69	0.73
1:D:342:LEU:HD12	1:D:358:LEU:HD12	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ASP:OD1	1:A:145:LEU:HD23	1.91	0.70
1:B:184:GLU:HG2	6:B:601:HOH:O	1.92	0.70
1:A:355:PHE:CE2	1:A:359:LEU:HD21	2.27	0.69
1:B:270:ASP:HB3	1:B:276:LEU:HD21	1.73	0.69
1:C:52:ASP:OD2	1:C:55:VAL:HG23	1.95	0.67
1:C:342:LEU:HD12	1:C:358:LEU:HD12	1.75	0.67
1:C:275:ILE:HD12	1:C:275:ILE:H	1.60	0.65
1:D:270:ASP:HB3	1:D:276:LEU:HD21	1.79	0.63
1:C:117:ALA:HB1	1:C:355:PHE:CZ	2.35	0.61
1:B:52:ASP:OD2	1:B:55:VAL:HG23	2.01	0.60
1:A:52:ASP:OD2	1:A:55:VAL:HG23	2.02	0.60
1:C:270:ASP:HB3	1:C:276:LEU:HD21	1.86	0.58
1:A:275:ILE:HD12	1:A:275:ILE:H	1.69	0.57
1:A:148:PRO:HG2	1:A:346:GLU:CG	2.34	0.57
1:D:52:ASP:OD2	1:D:55:VAL:HG23	2.05	0.56
1:D:124:ALA:HB2	1:D:134:VAL:HG21	1.86	0.56
1:A:11:LEU:HD12	1:A:11:LEU:C	2.30	0.56
1:C:117:ALA:HB1	1:C:355:PHE:HZ	1.72	0.55
1:D:11:LEU:C	1:D:11:LEU:HD12	2.32	0.54
1:A:121:VAL:HG21	1:A:355:PHE:CE2	2.43	0.53
1:A:270:ASP:HB3	1:A:276:LEU:HD21	1.90	0.52
1:C:11:LEU:C	1:C:11:LEU:HD12	2.36	0.51
1:A:346:GLU:CD	1:A:351:LYS:HE2	2.36	0.51
1:C:167:ILE:HD11	1:C:197:MET:HE3	1.92	0.50
1:D:217:ILE:HD12	1:D:252:LYS:HB3	1.94	0.50
1:B:127:MET:SD	1:B:132:ILE:HD13	2.51	0.50
1:B:11:LEU:HD12	1:B:11:LEU:C	2.36	0.49
1:C:289:GLU:OE1	1:C:292:LYS:NZ	2.46	0.48
1:B:167:ILE:HD11	1:B:197:MET:HE3	1.95	0.48
1:B:69:SER:OG	4:D:502:PO4:O1	2.31	0.47
1:A:179:ARG:HG2	1:A:180:TRP:N	2.29	0.47
1:A:324:ARG:HD3	6:A:616:HOH:O	2.15	0.47
1:C:90:PRO:HA	1:C:93:GLN:HB2	1.96	0.47
1:C:289:GLU:CD	1:C:292:LYS:NZ	2.73	0.46
1:A:112:GLY:HA2	1:A:139:LYS:HE3	1.97	0.46
1:D:167:ILE:HD11	1:D:197:MET:HE3	1.97	0.45
1:B:174:SER:O	1:B:178:PRO:HA	2.16	0.45
1:B:342:LEU:HD22	1:B:358:LEU:HD12	1.97	0.45
1:D:174:SER:O	1:D:178:PRO:HA	2.17	0.45
1:B:148:PRO:HD2	1:B:346:GLU:HG2	1.99	0.45
1:B:138:PRO:HB2	1:B:145:LEU:HD11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:ASP:HB2	1:B:271:PRO:CD	2.46	0.45
1:A:174:SER:O	1:A:178:PRO:HA	2.17	0.44
1:D:138:PRO:HD2	1:D:343:ILE:O	2.18	0.44
1:A:376:GLN:HG2	6:C:647:HOH:O	2.17	0.44
1:A:110:THR:O	1:A:136:SER:HA	2.18	0.43
1:C:89:SER:O	1:C:93:GLN:HG3	2.19	0.43
1:A:83:ARG:HH12	3:A:502:PPV:P2	2.42	0.43
1:C:180:TRP:HA	1:C:241:GLY:O	2.19	0.43
1:B:208:ILE:O	1:B:211:GLU:HG2	2.20	0.42
1:A:208:ILE:O	1:A:211:GLU:HG2	2.19	0.42
1:B:136:SER:O	1:B:342:LEU:HA	2.19	0.42
1:B:390:LYS:HG3	1:B:426:GLU:HG3	2.02	0.42
1:A:139:LYS:O	1:A:140:THR:HB	2.20	0.41
1:A:114:ASP:OD1	1:A:145:LEU:CD2	2.64	0.41
1:B:270:ASP:HB2	1:B:271:PRO:HD2	2.02	0.41
1:A:118:SER:O	1:A:121:VAL:HG22	2.20	0.41
1:C:135:ILE:CG2	1:C:343:ILE:HG12	2.50	0.41
1:A:36:TRP:CD1	1:A:36:TRP:N	2.88	0.41
1:A:188:ARG:HG2	1:A:247:GLU:HG3	2.02	0.41
1:B:37:LYS:HE2	1:B:62:ASP:OD1	2.21	0.40
1:B:143:ASN:HB2	1:B:156:PHE:CD1	2.56	0.40
1:A:148:PRO:HG2	1:A:346:GLU:CD	2.46	0.40
1:A:183:VAL:HA	1:A:304:LYS:O	2.21	0.40
1:B:97:ARG:HA	1:B:127:MET:HE1	2.04	0.40
1:D:141:ILE:HD11	1:D:159:ALA:HB2	2.04	0.40
1:B:139:LYS:HD2	1:B:139:LYS:C	2.45	0.40
1:A:164:MET:HE3	1:A:200:ALA:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	413/434 (95%)	407 (98%)	6 (2%)	0	100	100
1	B	421/434 (97%)	414 (98%)	7 (2%)	0	100	100
1	C	421/434 (97%)	416 (99%)	5 (1%)	0	100	100
1	D	414/434 (95%)	408 (99%)	6 (1%)	0	100	100
All	All	1669/1736 (96%)	1645 (99%)	24 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	337/355 (95%)	336 (100%)	1 (0%)	86	91
1	B	344/355 (97%)	342 (99%)	2 (1%)	78	84
1	C	344/355 (97%)	342 (99%)	2 (1%)	78	84
1	D	336/355 (95%)	334 (99%)	2 (1%)	78	84
All	All	1361/1420 (96%)	1354 (100%)	7 (0%)	81	87

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	THR
1	B	77	THR
1	B	300	ARG
1	C	77	THR
1	C	345	ARG
1	D	141	ILE
1	D	300	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	338	HIS

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Mol	Chain	Res	Type
1	B	338	HIS
1	B	349	GLN
1	C	264	ASN
1	C	274	HIS
1	C	419	HIS
1	D	264	ASN
1	D	354	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 6 are monoatomic - leaving 16 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
3	PPV	A	502	-	6,8,8	0.73	0	12,13,13	0.93	0
4	PO4	B	504	-	4,4,4	1.68	1 (25%)	6,6,6	0.81	0
4	PO4	B	505	-	4,4,4	1.73	1 (25%)	6,6,6	0.46	0
2	AMP	B	502	-	25,25,25	1.37	5 (20%)	37,38,38	2.16	11 (29%)
3	PPV	D	501	-	6,8,8	0.69	0	12,13,13	0.94	0
4	PO4	C	503	-	4,4,4	1.54	1 (25%)	6,6,6	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	AMP	B	501	-	25,25,25	1.45	4 (16%)	37,38,38	2.16	10 (27%)
4	PO4	D	502	-	4,4,4	1.39	1 (25%)	6,6,6	0.92	0
4	PO4	A	503	-	4,4,4	1.25	1 (25%)	6,6,6	0.84	0
3	PPV	C	502	-	6,8,8	0.66	0	12,13,13	1.17	0
2	AMP	C	501	-	25,25,25	1.44	3 (12%)	37,38,38	2.19	11 (29%)
4	PO4	A	504	-	4,4,4	1.74	1 (25%)	6,6,6	0.50	0
4	PO4	C	504	-	4,4,4	1.73	1 (25%)	6,6,6	0.49	0
3	PPV	B	503	-	6,8,8	0.59	0	12,13,13	0.96	0
4	PO4	D	503	-	4,4,4	1.70	1 (25%)	6,6,6	0.53	0
2	AMP	A	501	-	25,25,25	1.40	5 (20%)	37,38,38	2.32	12 (32%)

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
3	PPV	A	502	-	-	0/6/6/6	-
2	AMP	B	502	-	-	0/10/26/26	0/3/3/3
3	PPV	D	501	-	-	2/6/6/6	-
2	AMP	B	501	-	-	0/10/26/26	0/3/3/3
3	PPV	C	502	-	-	0/6/6/6	-
2	AMP	C	501	-	-	0/10/26/26	0/3/3/3
3	PPV	B	503	-	-	1/6/6/6	-
2	AMP	A	501	-	-	0/10/26/26	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	AMP	C5-C4	4.58	1.47	1.39
2	B	501	AMP	C5-C4	4.52	1.47	1.39
2	A	501	AMP	C5-C4	4.31	1.46	1.39
2	B	502	AMP	C5-C4	4.24	1.46	1.39
4	B	504	PO4	P-O1	3.13	1.57	1.50
4	B	505	PO4	P-O1	2.99	1.57	1.50
4	A	504	PO4	P-O1	2.98	1.57	1.50
4	C	504	PO4	P-O1	2.98	1.57	1.50
4	D	503	PO4	P-O1	2.90	1.57	1.50
2	C	501	AMP	C5-C6	2.83	1.48	1.41
4	C	503	PO4	P-O1	2.72	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	AMP	C5-C6	2.64	1.48	1.41
2	B	501	AMP	C8-N7	2.57	1.36	1.31
2	C	501	AMP	C8-N7	2.49	1.36	1.31
4	D	502	PO4	P-O1	2.46	1.56	1.50
2	B	502	AMP	C5-N7	-2.44	1.34	1.39
2	A	501	AMP	C5-C6	2.36	1.47	1.41
4	A	503	PO4	P-O1	2.35	1.56	1.50
2	B	502	AMP	C5-C6	2.34	1.47	1.41
2	B	502	AMP	C8-N7	2.24	1.36	1.31
2	A	501	AMP	C5-N7	-2.22	1.35	1.39
2	B	501	AMP	C5-N7	-2.14	1.35	1.39
2	A	501	AMP	C8-N7	2.11	1.35	1.31
2	A	501	AMP	O4'-C1'	2.03	1.46	1.42
2	B	502	AMP	C4-N9	-2.02	1.33	1.37

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	AMP	C5-C4-N3	-6.13	118.28	126.72
2	C	501	AMP	C5-C4-N3	-6.10	118.31	126.72
2	B	502	AMP	C5-C4-N3	-5.59	119.02	126.72
2	A	501	AMP	C5-C4-N3	-5.50	119.14	126.72
2	A	501	AMP	N3-C2-N1	-5.40	120.41	128.58
2	B	501	AMP	N3-C4-N9	5.38	136.32	127.17
2	C	501	AMP	N3-C4-N9	5.35	136.26	127.17
2	A	501	AMP	N3-C4-N9	5.27	136.13	127.17
2	B	502	AMP	N3-C4-N9	5.04	135.74	127.17
2	B	502	AMP	N3-C2-N1	-4.96	121.08	128.58
2	A	501	AMP	C2-N3-C4	4.48	122.78	111.83
2	B	502	AMP	C2-N3-C4	4.47	122.75	111.83
2	B	501	AMP	N3-C2-N1	-4.39	121.94	128.58
2	B	501	AMP	C2-N3-C4	4.36	122.48	111.83
2	C	501	AMP	C2-N3-C4	4.31	122.35	111.83
2	C	501	AMP	N3-C2-N1	-4.28	122.11	128.58
2	A	501	AMP	C4-N9-C8	4.18	110.13	105.74
2	C	501	AMP	C4-N9-C8	3.61	109.53	105.74
2	B	501	AMP	C4-N9-C8	3.47	109.38	105.74
2	B	502	AMP	C4-N9-C8	3.42	109.33	105.74
2	C	501	AMP	C4-C5-N7	-3.22	106.90	110.58
2	B	501	AMP	C4-C5-N7	-3.03	107.12	110.58
2	A	501	AMP	C2-N1-C6	2.84	123.39	118.73
2	A	501	AMP	N9-C8-N7	-2.82	109.94	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	AMP	C5-N7-C8	2.77	107.81	103.45
2	A	501	AMP	C4-C5-N7	-2.76	107.42	110.58
2	A	501	AMP	C5-N7-C8	2.76	107.78	103.45
2	B	501	AMP	C5-N7-C8	2.69	107.68	103.45
2	A	501	AMP	C2'-C1'-N9	2.63	119.84	113.30
2	C	501	AMP	N9-C8-N7	-2.54	110.33	113.94
2	B	501	AMP	N9-C8-N7	-2.48	110.42	113.94
2	B	502	AMP	C4-C5-N7	-2.37	107.87	110.58
2	B	502	AMP	O3P-P-O2P	2.36	116.64	107.80
2	B	502	AMP	C6-C5-N7	2.26	136.45	132.09
2	B	502	AMP	N9-C8-N7	-2.22	110.78	113.94
2	A	501	AMP	C6-C5-N7	2.21	136.34	132.09
2	A	501	AMP	N6-C6-N1	2.19	123.25	118.38
2	B	502	AMP	C5-N7-C8	2.11	106.77	103.45
2	C	501	AMP	N6-C6-N1	2.11	123.07	118.38
2	B	502	AMP	C5-C6-N6	-2.11	118.07	123.29
2	C	501	AMP	C6-C5-N7	2.10	136.15	132.09
2	C	501	AMP	C2-N1-C6	2.08	122.15	118.73
2	B	501	AMP	C6-C5-N7	2.08	136.10	132.09
2	B	501	AMP	N6-C6-N1	2.02	122.87	118.38

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	501	PPV	P2-OPP-P1-O21
3	D	501	PPV	P2-OPP-P1-O31
3	B	503	PPV	P2-OPP-P1-O11

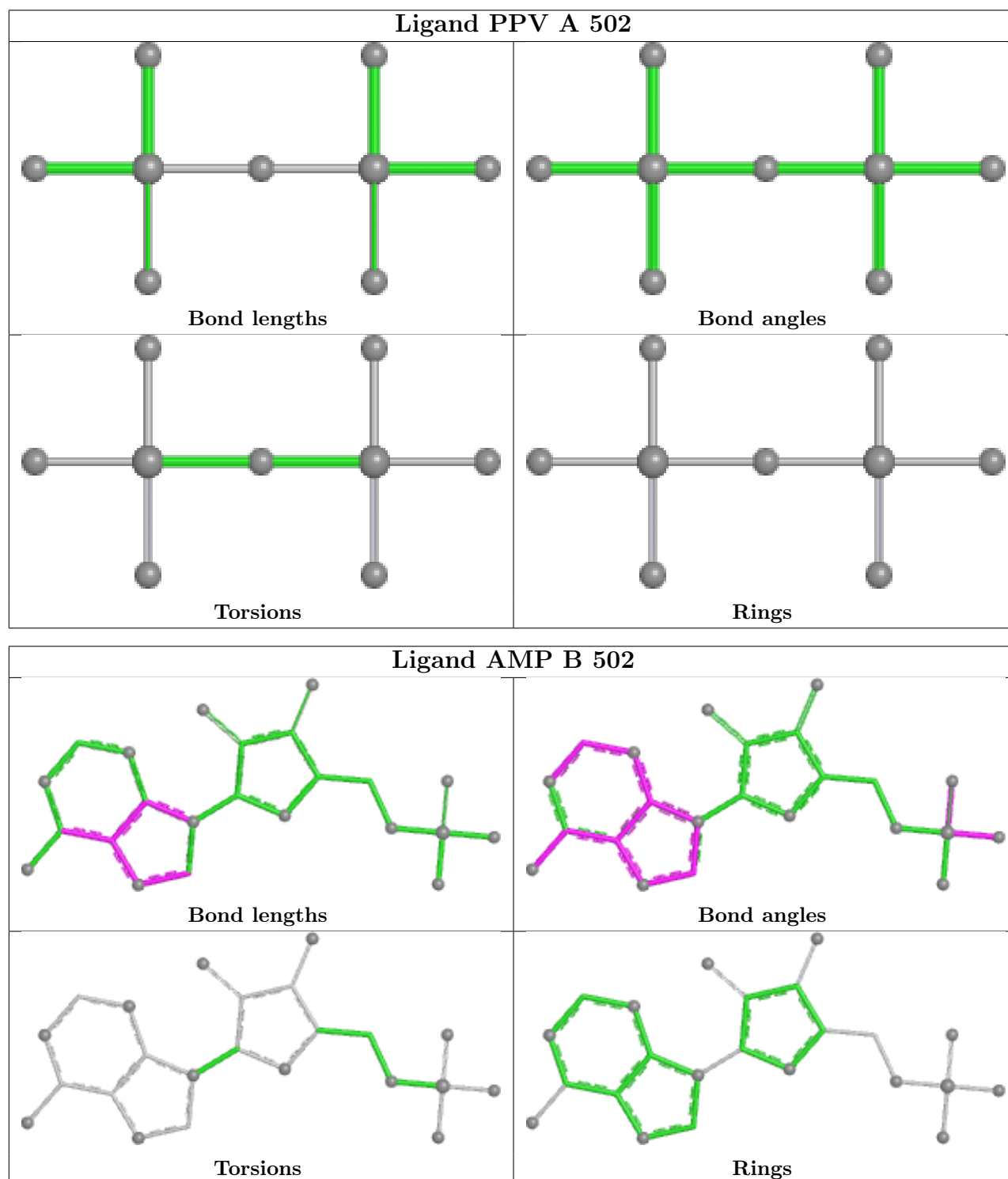
There are no ring outliers.

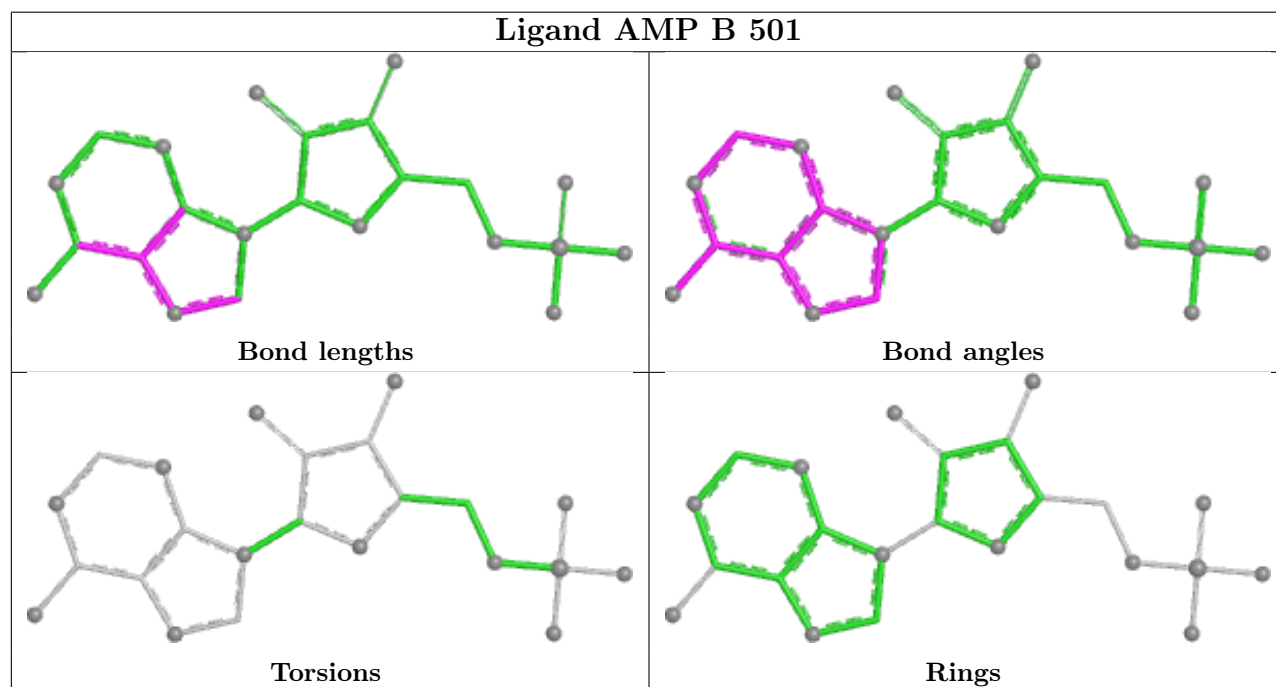
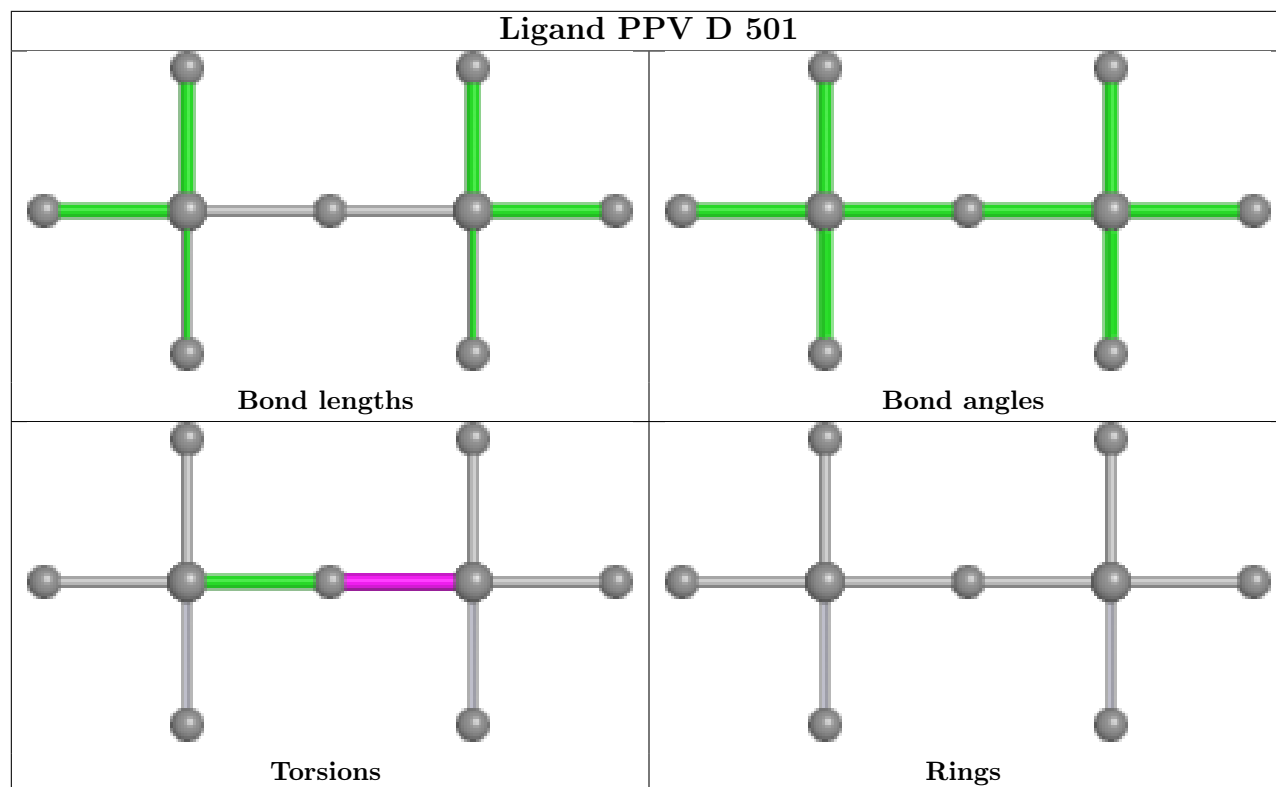
2 monomers are involved in 2 short contacts:

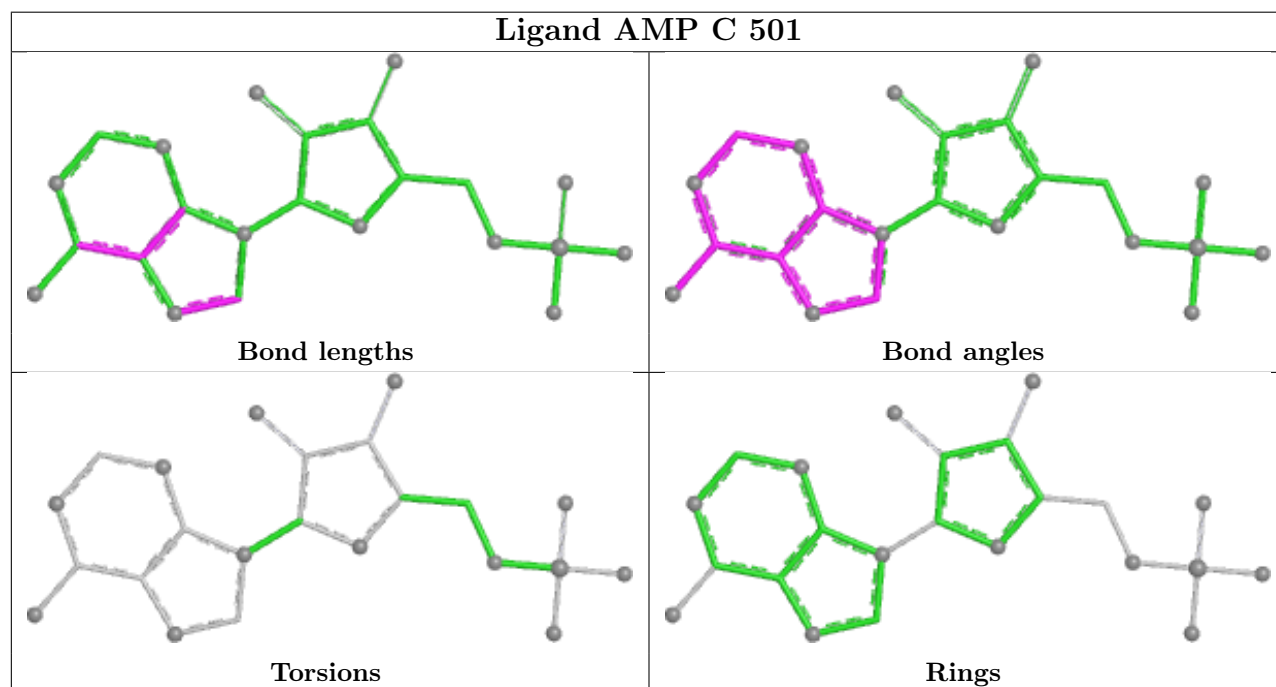
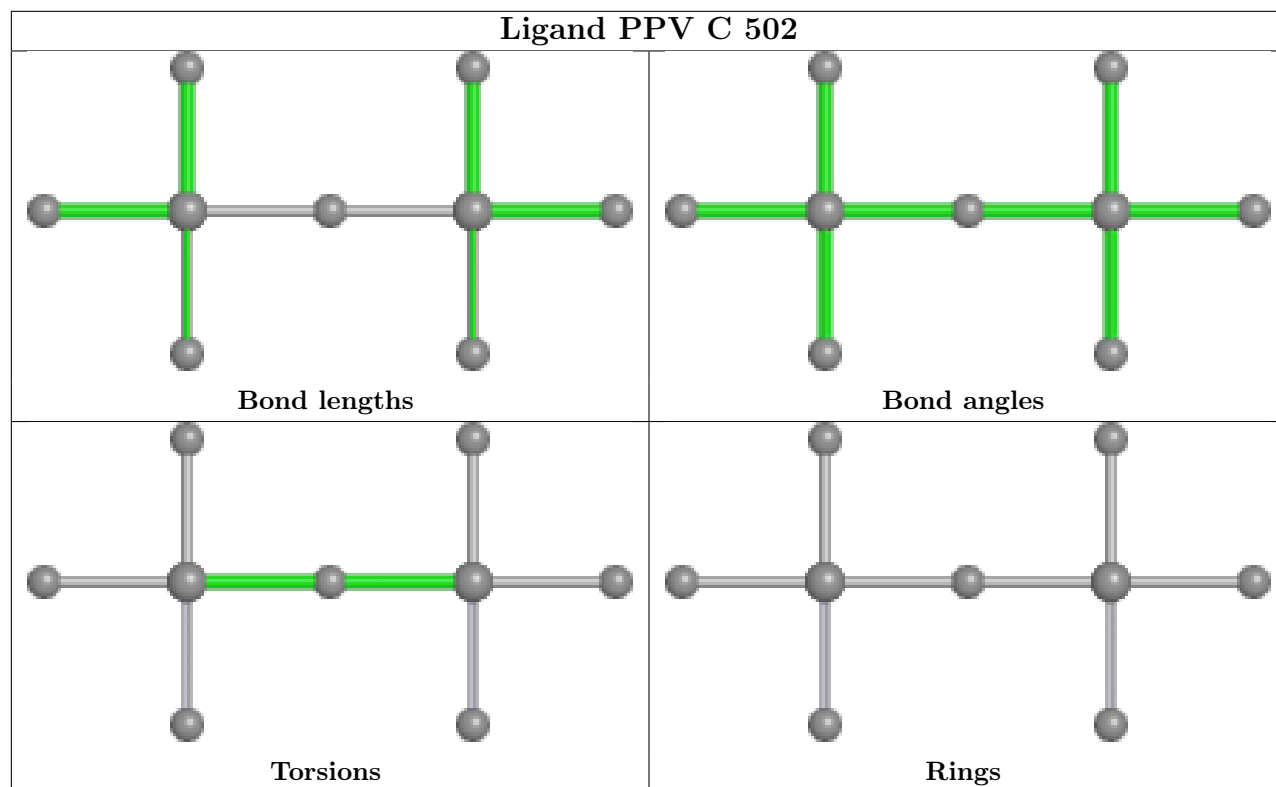
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	PPV	1	0
4	D	502	PO4	1	0

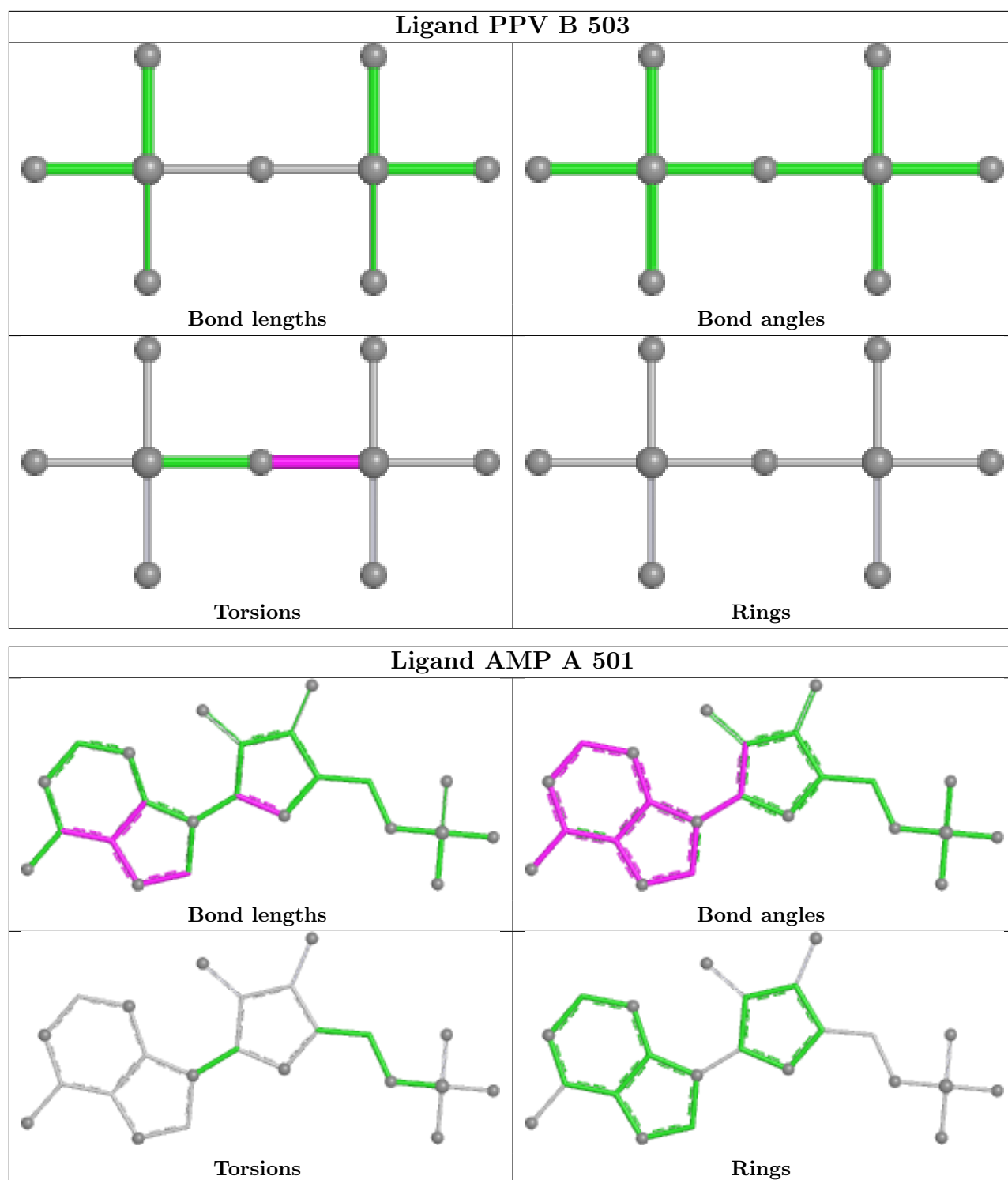
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	417/434 (96%)	0.43	33 (7%) 18 20	35, 54, 110, 153	0
1	B	423/434 (97%)	0.30	14 (3%) 49 53	35, 61, 100, 150	0
1	C	423/434 (97%)	0.24	18 (4%) 40 45	35, 56, 97, 131	0
1	D	418/434 (96%)	0.27	20 (4%) 35 40	37, 64, 107, 145	0
All	All	1681/1736 (96%)	0.31	85 (5%) 33 37	35, 60, 105, 153	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	142	ASP	5.7
1	A	346	GLU	5.5
1	C	88	LYS	4.8
1	D	368	THR	4.8
1	A	151	GLN	4.1
1	C	263	GLY	4.0
1	A	348	GLY	3.7
1	C	362	ALA	3.7
1	A	145	LEU	3.6
1	C	91	GLU	3.5
1	D	363	THR	3.5
1	A	126	GLY	3.4
1	A	355	PHE	3.4
1	D	140	THR	3.4
1	D	275	ILE	3.4
1	A	147	LEU	3.4
1	D	362	ALA	3.3
1	D	358	LEU	3.3
1	C	279	ASP	3.3
1	D	366	VAL	3.2
1	D	259	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	367	ARG	3.2
1	C	150	ASP	3.1
1	D	145	LEU	3.1
1	C	355	PHE	3.1
1	A	349	GLN	3.1
1	B	390	LYS	3.0
1	A	146	PRO	3.0
1	B	279	ASP	3.0
1	B	149	ALA	3.0
1	A	347	ASN	2.9
1	B	145	LEU	2.9
1	D	359	LEU	2.8
1	A	144	ASP	2.8
1	A	148	PRO	2.8
1	D	355	PHE	2.7
1	A	138	PRO	2.7
1	A	53	VAL	2.7
1	A	152	SER	2.6
1	D	114	ASP	2.6
1	C	101	ARG	2.6
1	C	149	ALA	2.6
1	A	114	ASP	2.6
1	A	141	ILE	2.6
1	A	132	ILE	2.6
1	C	359	LEU	2.6
1	C	308	TYR	2.5
1	B	397	ASP	2.5
1	B	394	GLU	2.4
1	D	361	PRO	2.4
1	C	422	ASP	2.4
1	A	90	PRO	2.4
1	D	147	LEU	2.3
1	D	141	ILE	2.3
1	B	268	PRO	2.3
1	B	141	ILE	2.3
1	A	140	THR	2.3
1	C	361	PRO	2.3
1	A	358	LEU	2.3
1	C	92	LEU	2.3
1	C	262	PHE	2.2
1	A	222	VAL	2.2
1	B	55	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	292	LYS	2.2
1	D	115	ASP	2.2
1	B	147	LEU	2.2
1	B	275	ILE	2.2
1	D	364	GLY	2.2
1	C	214	GLN	2.2
1	D	265	ARG	2.1
1	A	396	LYS	2.1
1	B	374	THR	2.1
1	C	390	LYS	2.1
1	B	153	THR	2.1
1	C	90	PRO	2.1
1	A	265	ARG	2.1
1	A	273	GLY	2.1
1	A	7	VAL	2.1
1	A	149	ALA	2.1
1	A	92	LEU	2.1
1	B	276	LEU	2.1
1	A	394	GLU	2.1
1	A	150	ASP	2.0
1	A	367	ARG	2.0
1	A	274	HIS	2.0

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
4	PO4	A	504	5/5	0.64	0.10	101,106,126,127	0

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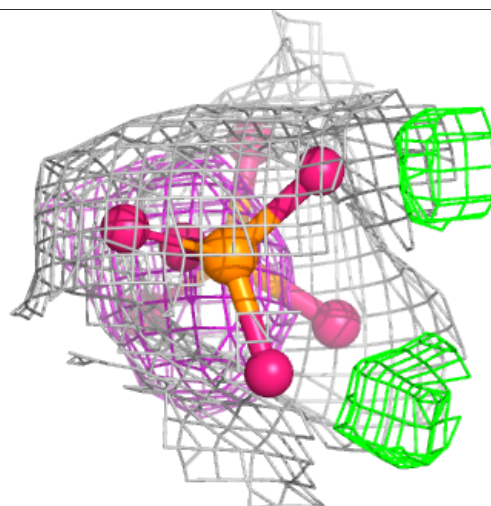
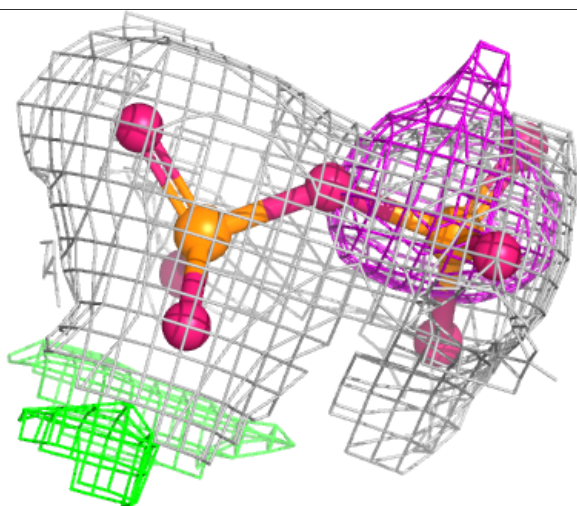
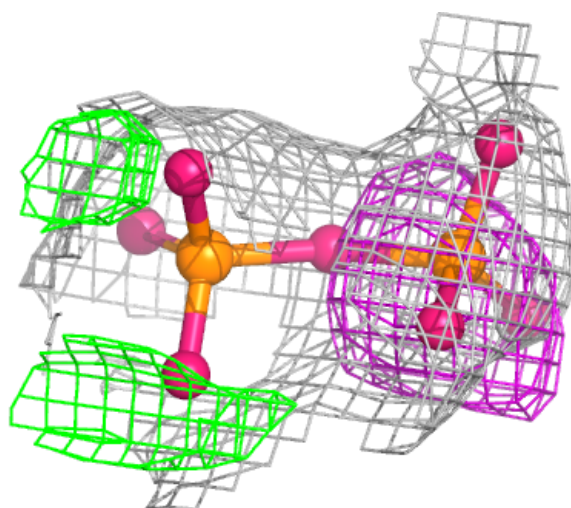
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PPV	B	503	9/9	0.71	0.12	68,79,82,85	0
3	PPV	C	502	9/9	0.74	0.12	70,86,89,93	0
3	PPV	D	501	9/9	0.77	0.10	77,87,94,98	0
2	AMP	C	501	23/23	0.81	0.10	58,75,94,99	0
2	AMP	B	501	23/23	0.82	0.10	61,74,92,97	0
3	PPV	A	502	9/9	0.83	0.10	68,84,94,109	0
4	PO4	C	504	5/5	0.85	0.09	76,80,85,98	0
4	PO4	D	503	5/5	0.85	0.07	91,93,103,113	0
2	AMP	B	502	23/23	0.86	0.09	53,62,71,76	0
4	PO4	B	505	5/5	0.87	0.08	86,88,108,117	0
2	AMP	A	501	23/23	0.91	0.08	39,55,67,70	0
5	CL	A	505	1/1	0.91	0.12	69,69,69,69	0
5	CL	B	506	1/1	0.93	0.09	66,66,66,66	0
4	PO4	B	504	5/5	0.95	0.07	54,55,57,57	0
5	CL	B	507	1/1	0.95	0.07	58,58,58,58	0
5	CL	D	504	1/1	0.95	0.07	74,74,74,74	0
4	PO4	D	502	5/5	0.96	0.06	56,56,58,59	0
4	PO4	C	503	5/5	0.96	0.08	51,52,57,61	0
5	CL	A	506	1/1	0.97	0.11	70,70,70,70	0
5	CL	D	505	1/1	0.97	0.07	60,60,60,60	0
4	PO4	A	503	5/5	0.98	0.06	47,48,54,54	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.

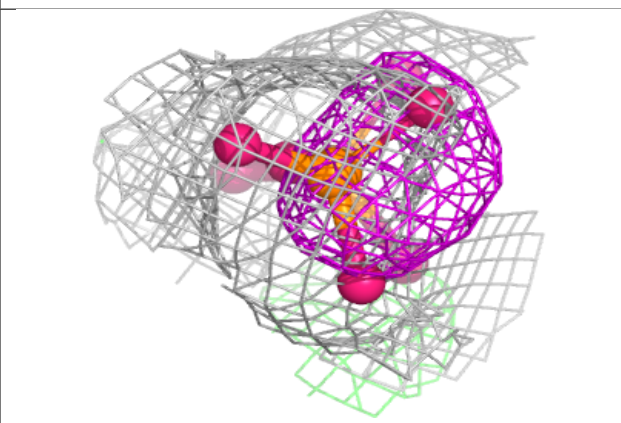
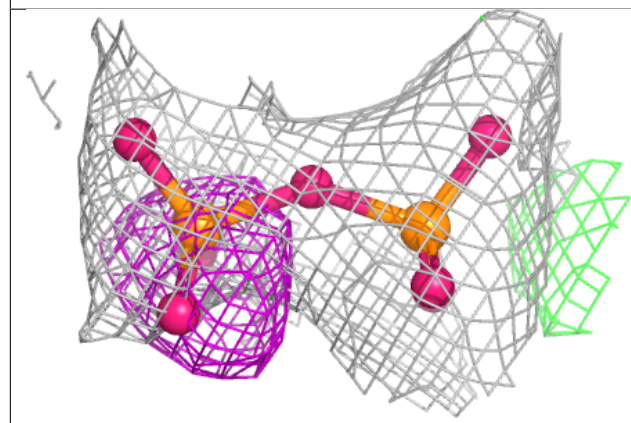
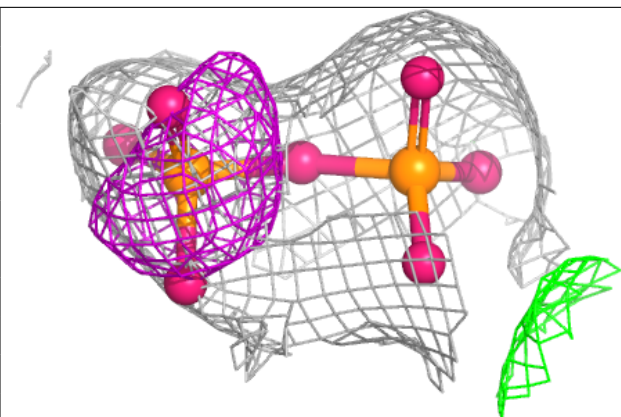
Electron density around PPV B 503:

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

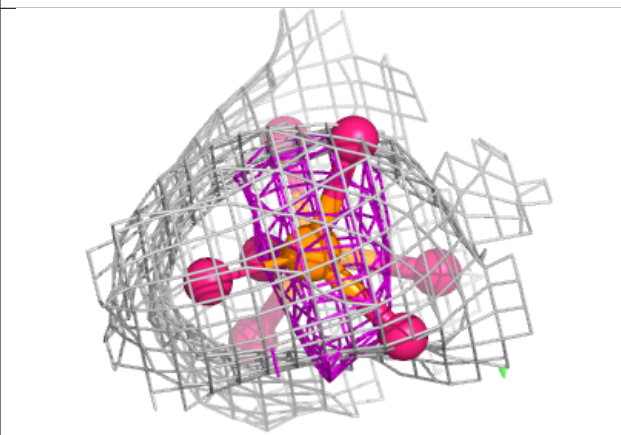
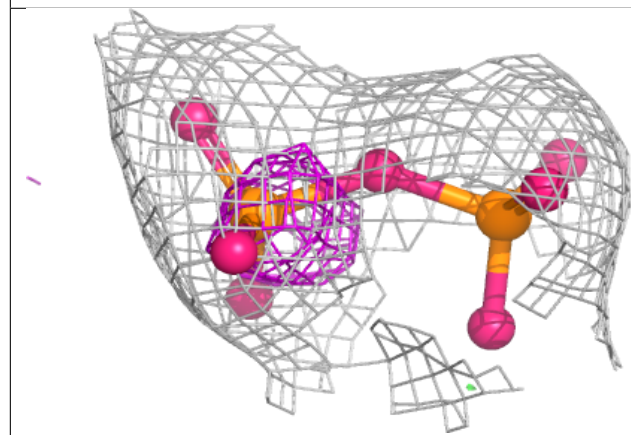
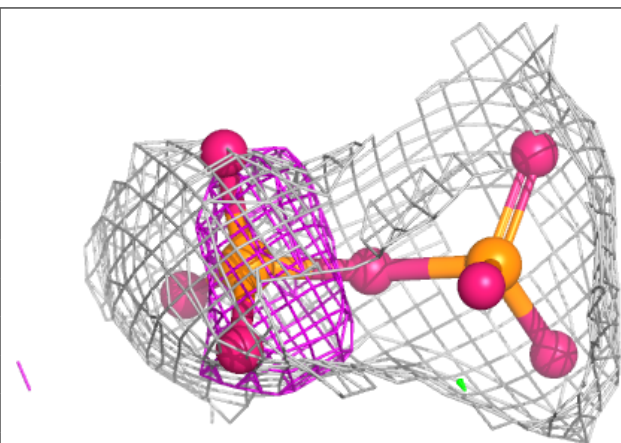


Electron density around PPV C 502:

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

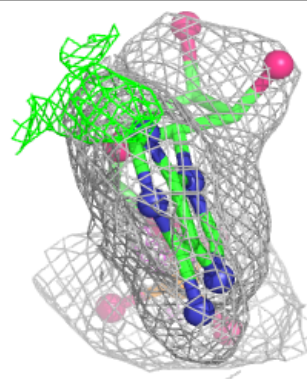
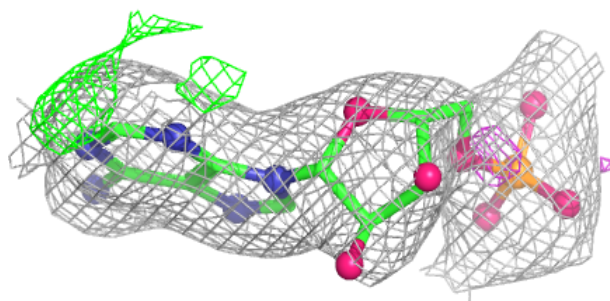
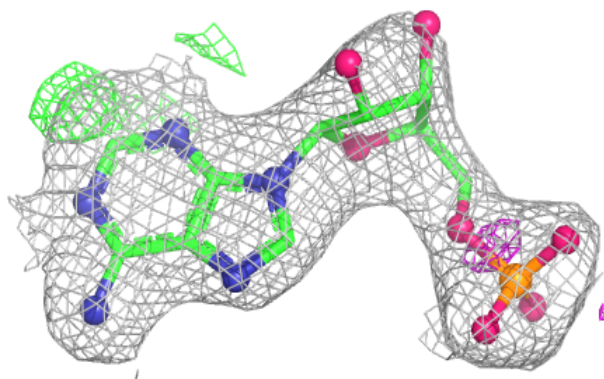
**Electron density around PPV D 501:**

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

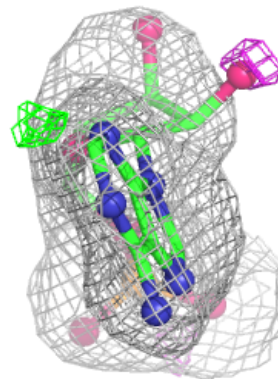
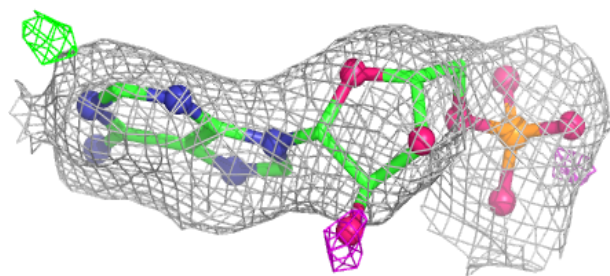
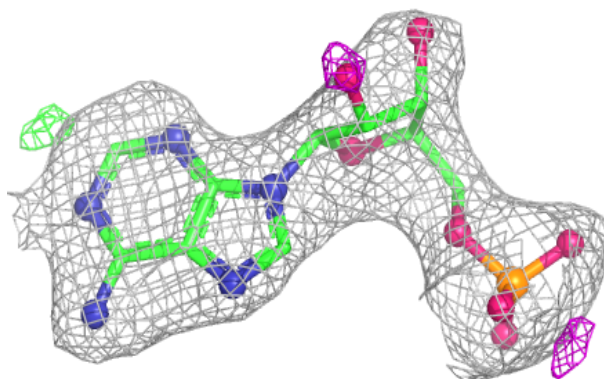


Electron density around AMP C 501:

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

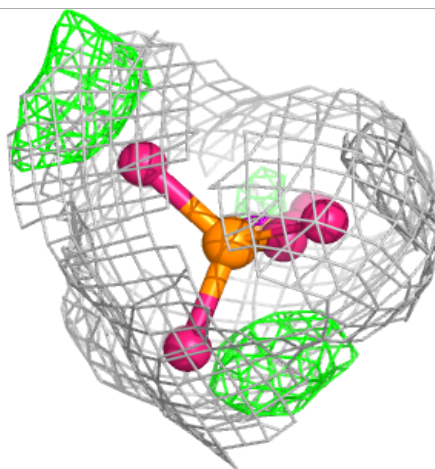
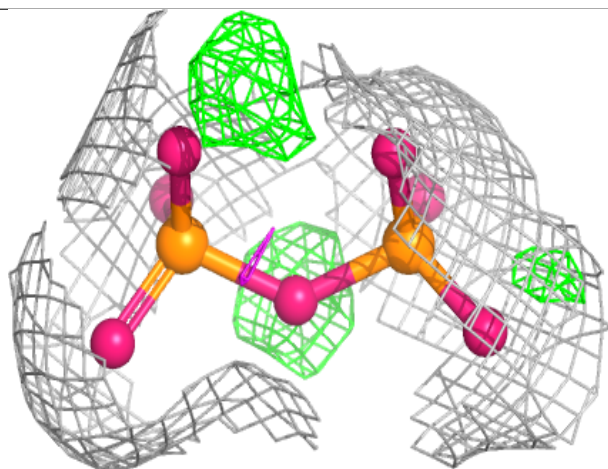
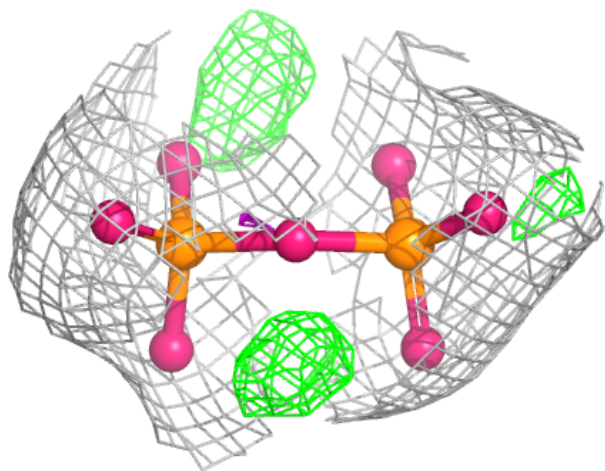
**Electron density around AMP B 501:**

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



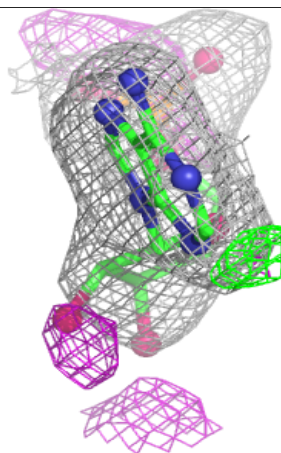
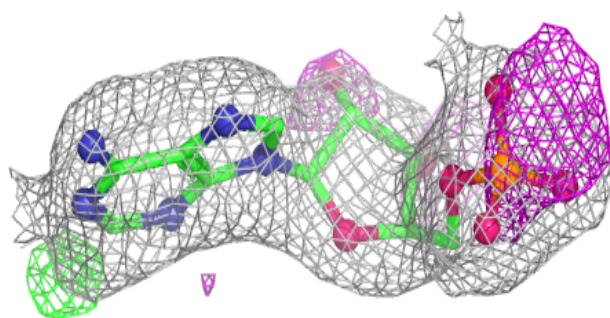
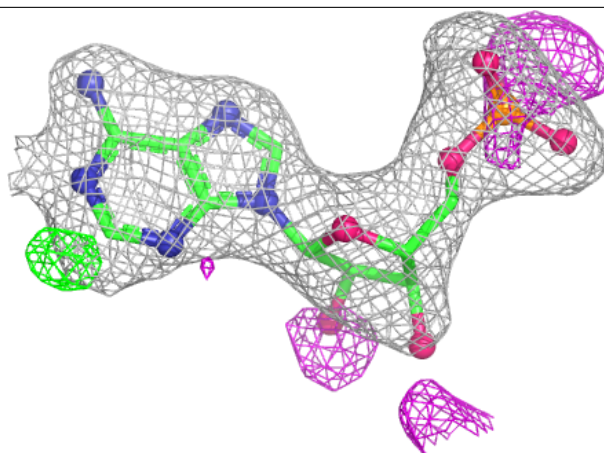
Electron density around PPV A 502:

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

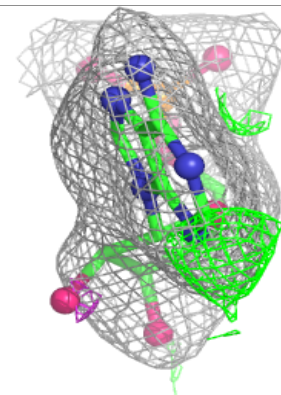
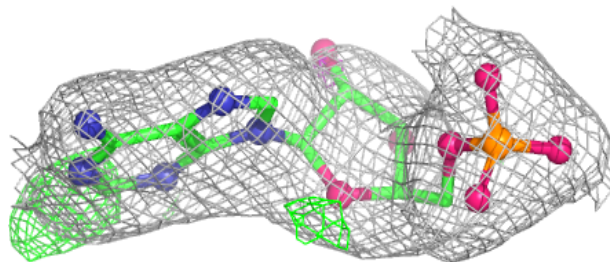
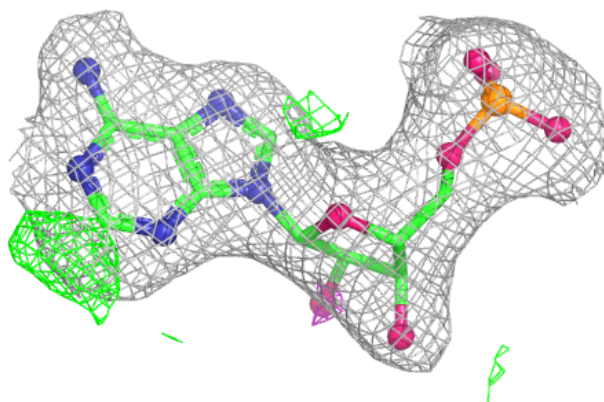


Electron density around AMP B 502:

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

**Electron density around AMP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.