



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 14, 2020 – 07:59 am BST

PDB ID : 1RFU
Title : Crystal structure of pyridoxal kinase complexed with ADP and PLP
Authors : Liang, D.-C.; Jiang, T.; Li, M.-H.
Deposited on : 2003-11-10
Resolution : 2.80 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

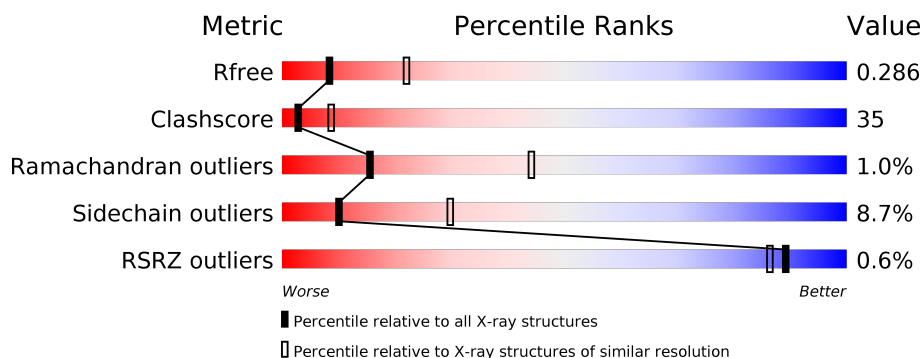
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 on 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	312	
1	B	312	
1	C	312	
1	D	312	
1	E	312	
1	F	312	

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Mol	Chain	Length	Quality of chain
1	G	312	<div><div></div><div>42%</div><div>53%</div><div>5%</div></div>
1	H	312	<div>%<div><div></div><div>37%</div><div>58%</div><div>5%</div></div></div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 20123 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 pyridoxal kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	312	Total	C	N	O	S	0	0	0
			2439	1532	427	463	17			
1	B	312	Total	C	N	O	S	0	0	0
			2439	1532	427	463	17			
1	C	312	Total	C	N	O	S	0	0	0
			2439	1532	427	463	17			
1	D	312	Total	C	N	O	S	0	0	0
			2439	1532	427	463	17			
1	E	312	Total	C	N	O	S	0	0	0
			2439	1532	427	463	17			
1	F	312	Total	C	N	O	S	0	0	0
			2439	1532	427	463	17			
1	G	312	Total	C	N	O	S	0	0	0
			2439	1532	427	463	17			
1	H	312	Total	C	N	O	S	0	0	0
			2439	1532	427	463	17			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

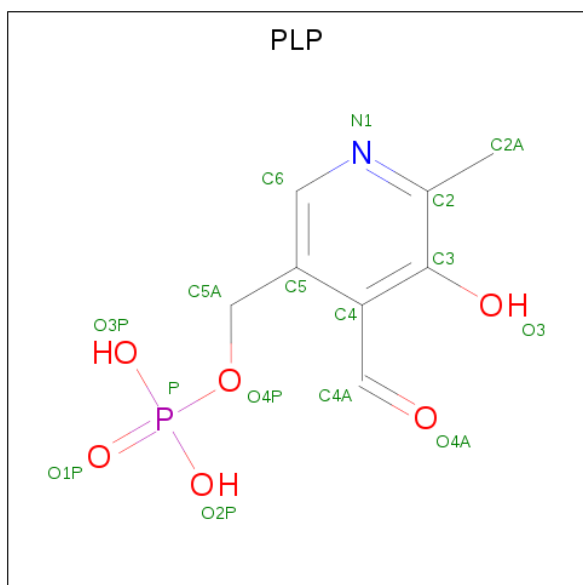
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	E	1	Total	Zn	0	0
			1	1		
2	H	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

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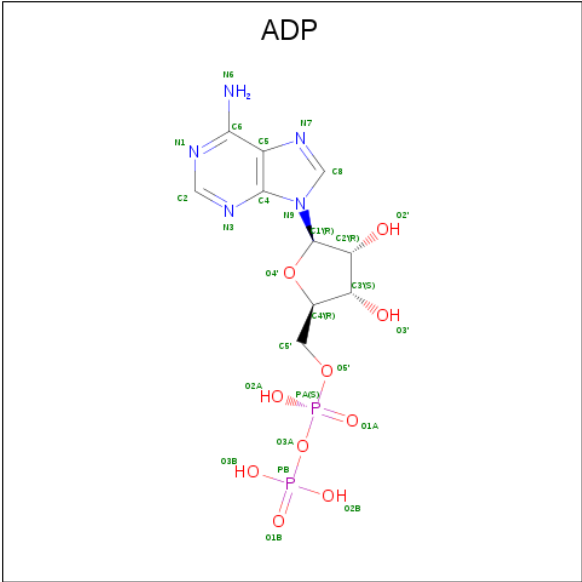
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	F	1	Total	Zn	0	0
			1	1		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	E	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	F	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	G	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	H	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	73	Total	O	0	0
			73	73		
5	B	54	Total	O	0	0
			54	54		
5	C	20	Total	O	0	0
			20	20		
5	D	9	Total	O	0	0
			9	9		

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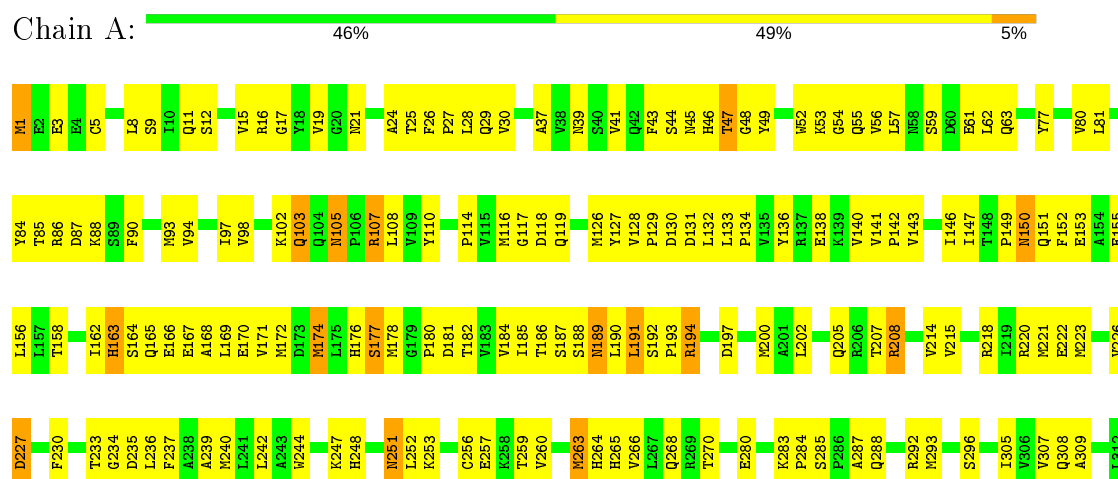
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	41	Total 41	O 41	0	0
5	F	37	Total 37	O 37	0	0
5	G	21	Total 21	O 21	0	0
5	H	12	Total 12	O 12	0	0

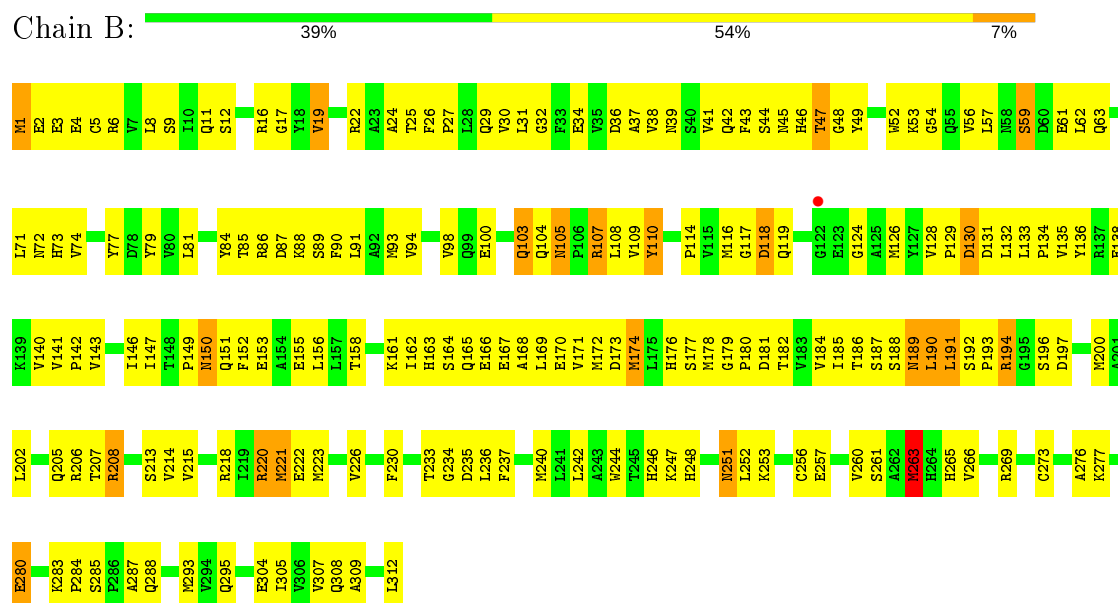
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

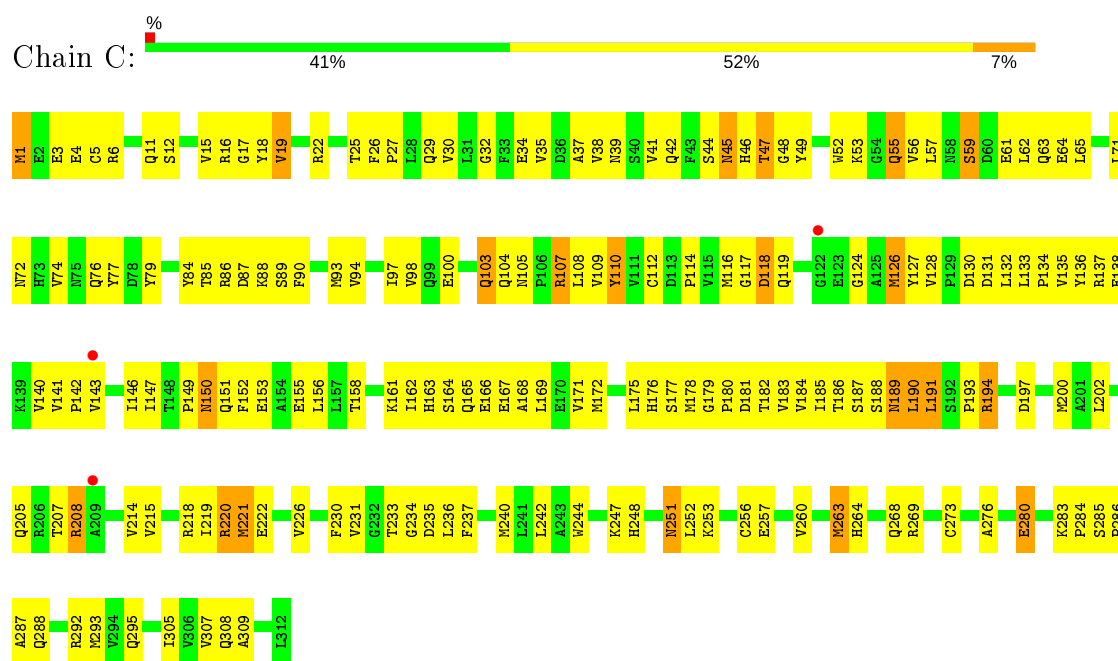
- Molecule 1: pyridoxal kinase



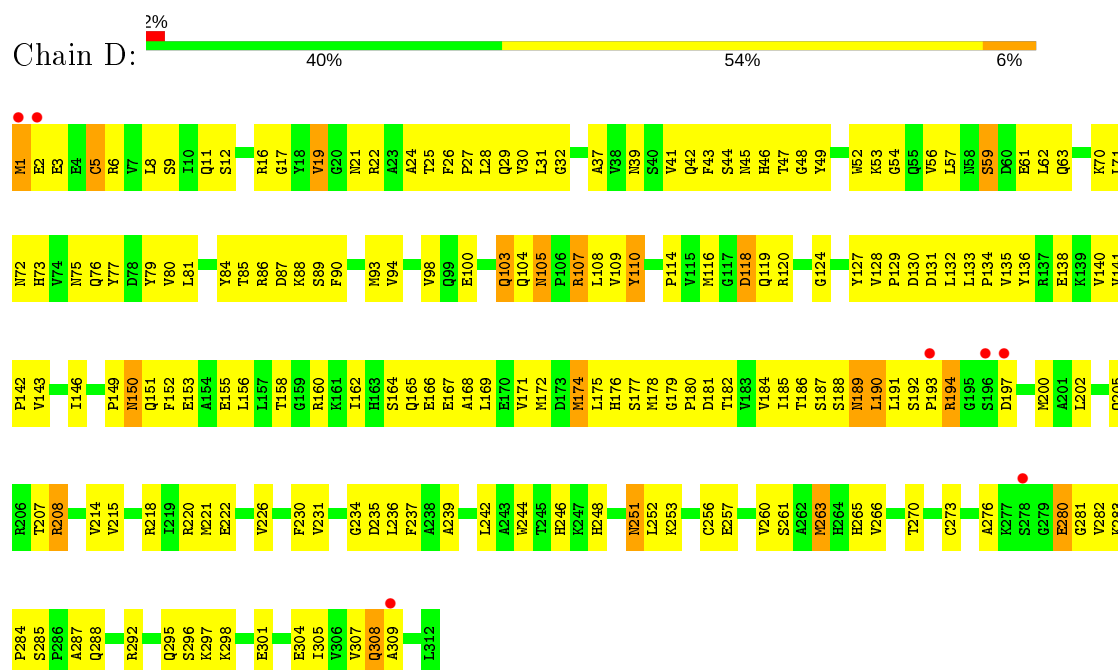
- Molecule 1: pyridoxal kinase



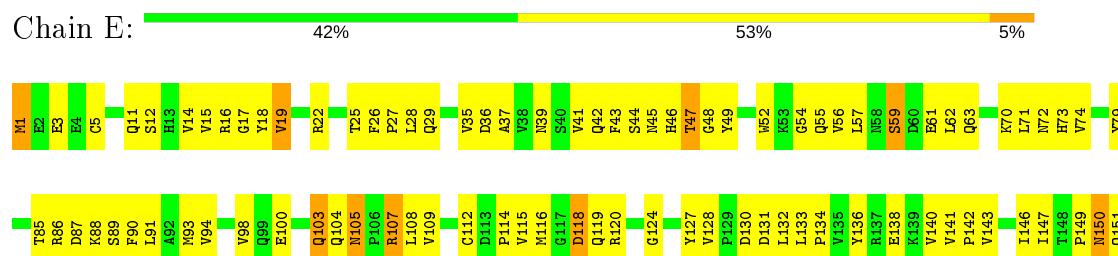
- Molecule 1: pyridoxal kinase



- Molecule 1: pyridoxal kinase



- Molecule 1: pyridoxal kinase



V282	M1	N72	I146	T207
K283	E2	H73	I147	R208
P284	E3		T148	V214
S285	E4	Q76	P149	V215
A287	C5	Y79	M150	R218
Q288	R6	V80	Q151	I219
		L81	F152	R220
R292	S9		E153	M221
M293	I10	T85	A154	E222
V294	Q11	R86	E155	M223
Q295	S12	D87	L156	V226
S296	S15	K88	L157	D227
K297	R16	S89	T158	I228
	G17	F90	G159	A228
I305	Y18	N93	R160	V229
V306	G20	V94	F161	F230
Q308	N21		I162	
A309	R22	V98	H163	T233
T310		Q99	S164	G234
V311	T25	E100	Q165	D235
L312	F26		E166	I236
	P27	Q103	E167	F237
	L28	Q104	A168	M238
	Q29	M105	L169	A239
	V30	P106	E170	P240
L31	L31	R107	V171	L241
E34		L108	M172	L242
		V109	M174	A243
		Y110	L175	V244
N39		H111	H176	
S40	N39	C112	S177	R247
V41	S40	D113	M178	H248
Q42	V41	P114	G179	
F43	Q42	V115	P180	N251
S44	F43	M116	D181	L252
N45	S44	C117	T182	K253
H46	N45	D118	V183	
T47	H46	Q119	V184	C256
G48	T47		I185	E257
Y49	G48	G122	T186	V260
S50	Y49		S187	
H51	S50	M126	S188	R263
M52	H51	Y127	N189	H264
K53	M52	V128	L190	H265
G54	K53	P129	L191	V266
Q55	G54	D130	S192	L267
V56	Q55	D131	P193	Q268
L57	V56	L132	R194	R269
N58	L57	L133		T270
S59	N58	P134	D197	
D60	S59	V135	Y198	C273
E61	D60	Y136	L199	
L62	E61	R137	M200	A276
Q63	L62	E138	A201	
	Q63		L202	G279
L69		V141	Q205	E280
K70	L69	P142	R206	G281
L71	K70	V143		

4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	109.09 Å 109.09 Å 284.27 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 19.94 – 2.80	Depositor EDS
% Data completeness (in resolution range)	87.5 (20.00-2.80) 56.7 (19.94-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 2.79 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.229 , 0.281 0.238 , 0.286	Depositor DCC
R_{free} test set	3623 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	56.6	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 28.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.40$	Xtriage
Estimated twinning fraction	0.488 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20123	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 87.15 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.5074e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, ADP, PLP

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	0.51	0/2484	0.74	1/3367 (0.0%)
1	B	0.54	0/2484	0.79	5/3367 (0.1%)
1	C	0.47	0/2484	0.74	3/3367 (0.1%)
1	D	0.45	0/2484	0.71	1/3367 (0.0%)
1	E	0.54	0/2484	0.76	1/3367 (0.0%)
1	F	0.55	0/2484	0.76	1/3367 (0.0%)
1	G	0.45	0/2484	0.71	1/3367 (0.0%)
1	H	0.44	0/2484	0.71	1/3367 (0.0%)
All	All	0.50	0/19872	0.74	14/26936 (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	E	0	1
1	F	0	2
1	H	0	2
All	All	0	5

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	220	ARG	NE-CZ-NH2	6.69	123.65	120.30
1	C	220	ARG	NE-CZ-NH2	6.28	123.44	120.30
1	F	178	MET	CG-SD-CE	6.12	110.00	100.20
1	B	221	MET	CG-SD-CE	6.12	109.99	100.20
1	C	126	MET	CG-SD-CE	6.12	109.99	100.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	18	TYR	Sidechain
1	F	127	TYR	Sidechain
1	F	18	TYR	Sidechain
1	H	127	TYR	Sidechain
1	H	18	TYR	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	2439	0	2442	176	0
1	B	2439	0	2442	200	0
1	C	2439	0	2442	198	0
1	D	2439	0	2442	182	0
1	E	2439	0	2442	172	0
1	F	2439	0	2442	180	0
1	G	2439	0	2442	163	0
1	H	2439	0	2442	209	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	15	0	7	2	0
3	B	15	0	6	1	0
3	C	15	0	6	1	0
3	D	15	0	7	1	0
3	E	15	0	6	1	0
3	F	15	0	7	2	0
3	G	15	0	6	1	0
3	H	15	0	7	1	0
4	A	27	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	27	0	12	2	0
4	C	27	0	12	1	0
4	D	27	0	12	1	0
4	E	27	0	12	1	0
4	F	27	0	12	2	0
4	G	27	0	12	1	0
4	H	27	0	12	2	0
5	A	73	0	0	4	0
5	B	54	0	0	5	0
5	C	20	0	0	2	0
5	D	9	0	0	2	0
5	E	41	0	0	3	0
5	F	37	0	0	5	0
5	G	21	0	0	2	0
5	H	12	0	0	3	0
All	All	20123	0	19684	1390	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 35.

The worst 5 of 1390 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:129:PRO:HG3	1:B:191:LEU:HB2	1.22	1.19
1:B:39:ASN:H	1:F:42:GLN:HE22	1.07	0.95
1:A:191:LEU:HB2	1:D:129:PRO:HG3	1.50	0.93
1:H:208:ARG:HH11	1:H:208:ARG:HG3	1.31	0.93
1:A:39:ASN:H	1:E:42:GLN:HE22	1.05	0.92

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	310/312 (99%)	279 (90%)	29 (9%)	2 (1%)	25	56
1	B	310/312 (99%)	276 (89%)	30 (10%)	4 (1%)	12	36
1	C	310/312 (99%)	272 (88%)	34 (11%)	4 (1%)	12	36
1	D	310/312 (99%)	274 (88%)	34 (11%)	2 (1%)	25	56
1	E	310/312 (99%)	274 (88%)	31 (10%)	5 (2%)	9	31
1	F	310/312 (99%)	274 (88%)	34 (11%)	2 (1%)	25	56
1	G	310/312 (99%)	275 (89%)	32 (10%)	3 (1%)	15	44
1	H	310/312 (99%)	271 (87%)	36 (12%)	3 (1%)	15	44
All	All	2480/2496 (99%)	2195 (88%)	260 (10%)	25 (1%)	15	44

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	191	LEU
1	D	191	LEU
1	H	191	LEU
1	B	191	LEU
1	C	191	LEU

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	273/273 (100%)	249 (91%)	24 (9%)	10	29
1	B	273/273 (100%)	249 (91%)	24 (9%)	10	29
1	C	273/273 (100%)	249 (91%)	24 (9%)	10	29
1	D	273/273 (100%)	249 (91%)	24 (9%)	10	29
1	E	273/273 (100%)	249 (91%)	24 (9%)	10	29
1	F	273/273 (100%)	251 (92%)	22 (8%)	11	33
1	G	273/273 (100%)	250 (92%)	23 (8%)	11	31
1	H	273/273 (100%)	248 (91%)	25 (9%)	9	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2184/2184 (100%)	1994 (91%)	190 (9%)	10	30

5 of 190 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	130	ASP
1	E	127	TYR
1	H	127	TYR
1	D	189	ASN
1	E	1	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	105	ASN
1	E	103	GLN
1	H	103	GLN
1	D	119	GLN
1	E	13	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 8 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	PLP	D	3401	2	15,15,16	1.62	2 (13%)	20,22,23	2.16	4 (20%)
4	ADP	A	402	2	24,29,29	1.19	2 (8%)	29,45,45	1.60	4 (13%)
4	ADP	B	1402	2	24,29,29	1.72	7 (29%)	29,45,45	1.55	3 (10%)
3	PLP	G	6401	2	15,15,16	1.73	3 (20%)	20,22,23	2.05	5 (25%)
3	PLP	C	2401	2	15,15,16	1.69	3 (20%)	20,22,23	2.01	5 (25%)
4	ADP	H	7402	2	24,29,29	1.68	6 (25%)	29,45,45	1.55	3 (10%)
4	ADP	E	4402	2	24,29,29	1.64	6 (25%)	29,45,45	1.53	3 (10%)
3	PLP	H	7401	2	15,15,16	1.55	3 (20%)	20,22,23	2.01	4 (20%)
3	PLP	A	401	2	15,15,16	2.02	3 (20%)	20,22,23	2.32	6 (30%)
4	ADP	F	5402	2	24,29,29	1.71	7 (29%)	29,45,45	1.57	3 (10%)
3	PLP	B	1401	2	15,15,16	1.59	3 (20%)	20,22,23	2.09	6 (30%)
4	ADP	C	2402	2	24,29,29	1.72	6 (25%)	29,45,45	1.55	2 (6%)
3	PLP	E	4401	2	15,15,16	1.54	2 (13%)	20,22,23	2.09	5 (25%)
4	ADP	G	6402	2	24,29,29	1.67	6 (25%)	29,45,45	1.53	3 (10%)
3	PLP	F	5401	2	15,15,16	1.65	2 (13%)	20,22,23	2.07	4 (20%)
4	ADP	D	3402	2	24,29,29	1.68	6 (25%)	29,45,45	1.57	3 (10%)

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	PLP	D	3401	2	-	2/6/6/8	0/1/1/1
4	ADP	A	402	2	-	7/12/32/32	0/3/3/3
4	ADP	B	1402	2	-	2/12/32/32	0/3/3/3
3	PLP	G	6401	2	-	2/6/6/8	0/1/1/1
3	PLP	C	2401	2	-	2/6/6/8	0/1/1/1
4	ADP	H	7402	2	-	2/12/32/32	0/3/3/3
4	ADP	E	4402	2	-	3/12/32/32	0/3/3/3
3	PLP	H	7401	2	-	2/6/6/8	0/1/1/1
3	PLP	A	401	2	-	4/6/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	F	5402	2	-	2/12/32/32	0/3/3/3
3	PLP	B	1401	2	-	1/6/6/8	0/1/1/1
4	ADP	C	2402	2	-	2/12/32/32	0/3/3/3
3	PLP	E	4401	2	-	1/6/6/8	0/1/1/1
4	ADP	G	6402	2	-	2/12/32/32	0/3/3/3
3	PLP	F	5401	2	-	2/6/6/8	0/1/1/1
4	ADP	D	3402	2	-	2/12/32/32	0/3/3/3

The worst 5 of 67 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	PLP	C5-C4	5.56	1.46	1.40
3	C	2401	PLP	C5-C4	4.35	1.45	1.40
3	D	3401	PLP	C5-C4	4.26	1.45	1.40
3	G	6401	PLP	C5-C4	4.12	1.45	1.40
3	B	1401	PLP	C5-C4	4.01	1.44	1.40

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3401	PLP	O4P-C5A-C5	6.99	122.67	109.35
4	D	3402	ADP	N3-C2-N1	-6.31	118.81	128.68
3	A	401	PLP	O4P-C5A-C5	6.29	121.33	109.35
3	G	6401	PLP	O4P-C5A-C5	6.25	121.27	109.35
4	A	402	ADP	N3-C2-N1	-6.25	118.91	128.68

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

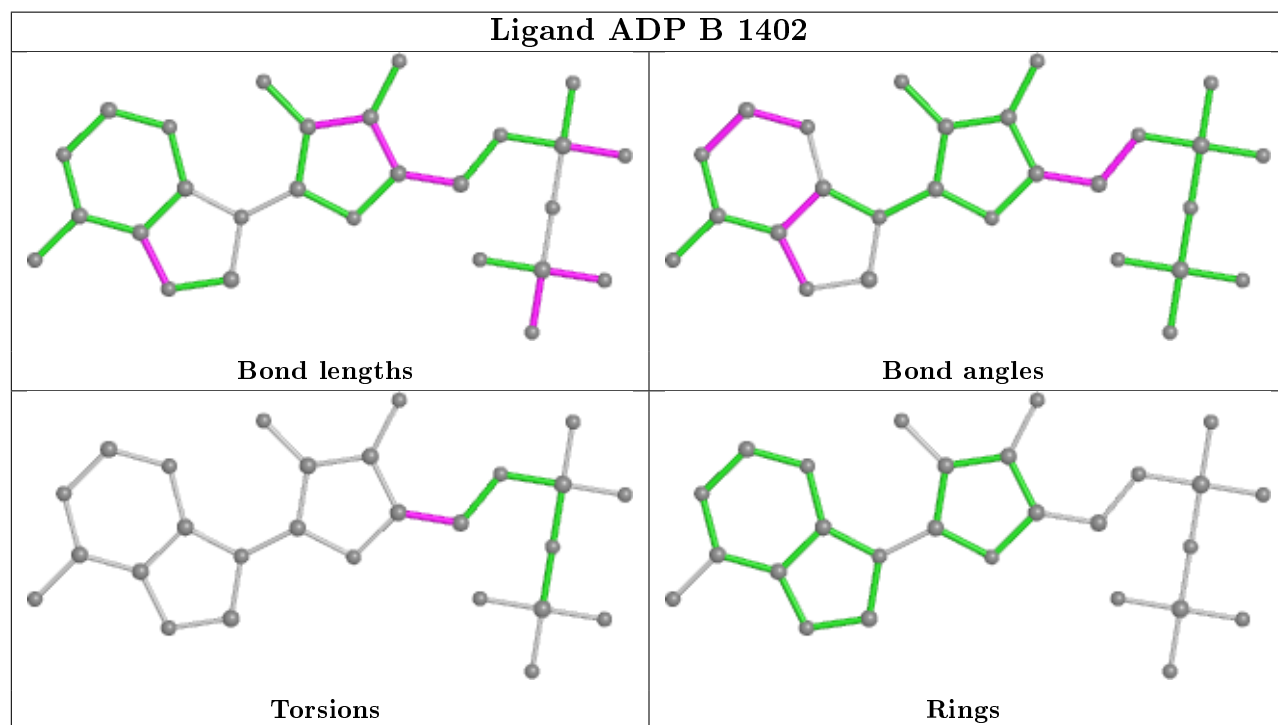
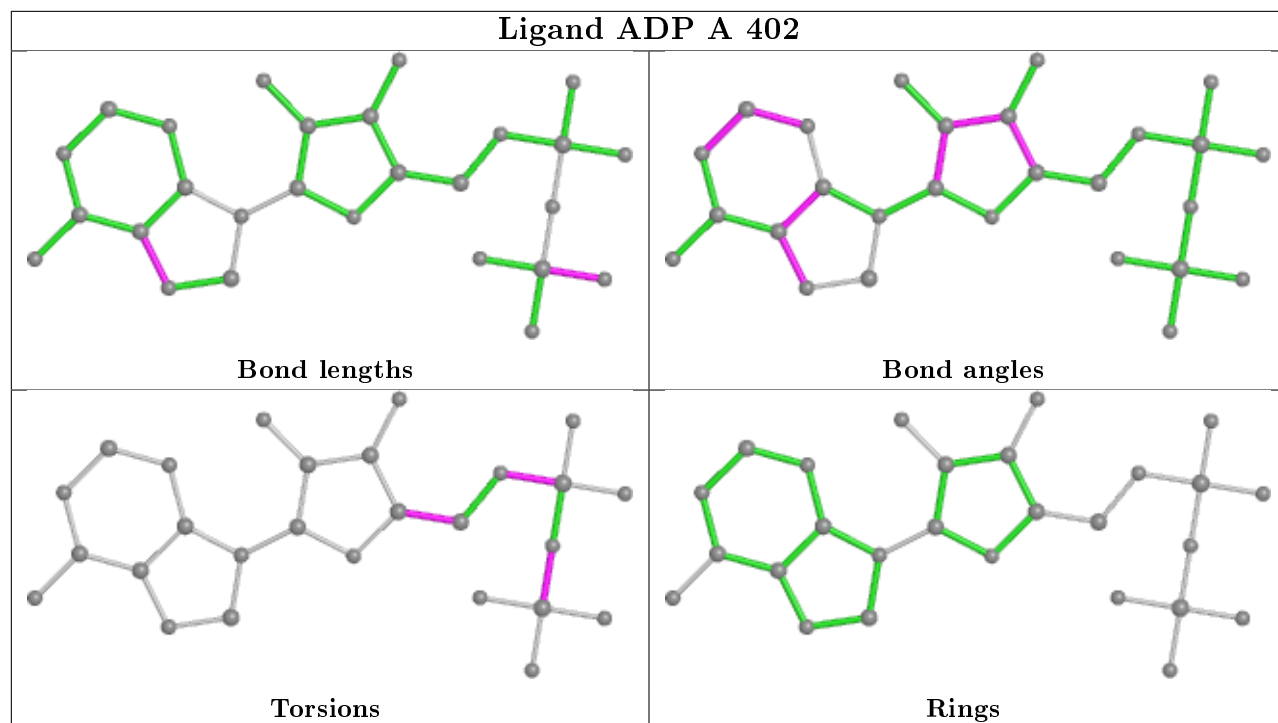
Mol	Chain	Res	Type	Atoms
4	G	6402	ADP	O4'-C4'-C5'-O5'
3	D	3401	PLP	C4-C5-C5A-O4P
4	A	402	ADP	C5'-O5'-PA-O3A
4	D	3402	ADP	O4'-C4'-C5'-O5'
3	G	6401	PLP	C4-C5-C5A-O4P

There are no ring outliers.

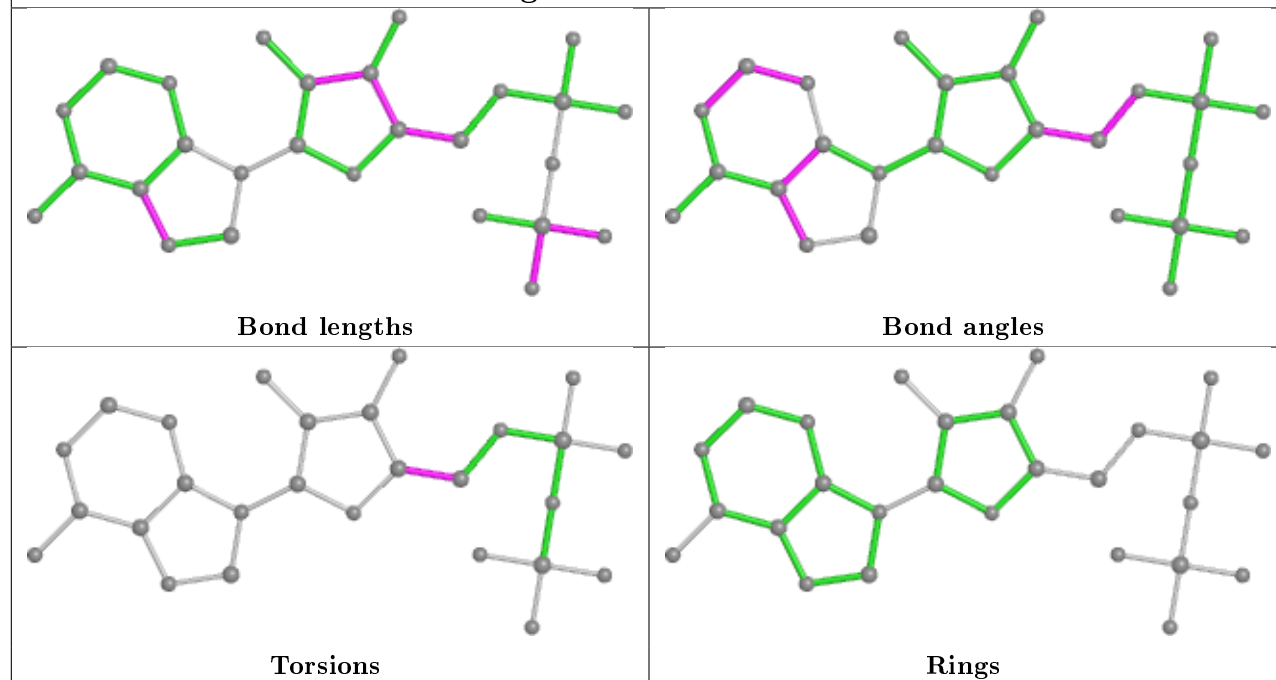
16 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	3401	PLP	1	0
4	A	402	ADP	3	0
4	B	1402	ADP	2	0
3	G	6401	PLP	1	0
3	C	2401	PLP	1	0
4	H	7402	ADP	2	0
4	E	4402	ADP	1	0
3	H	7401	PLP	1	0
3	A	401	PLP	2	0
4	F	5402	ADP	2	0
3	B	1401	PLP	1	0
4	C	2402	ADP	1	0
3	E	4401	PLP	1	0
4	G	6402	ADP	1	0
3	F	5401	PLP	2	0
4	D	3402	ADP	1	0

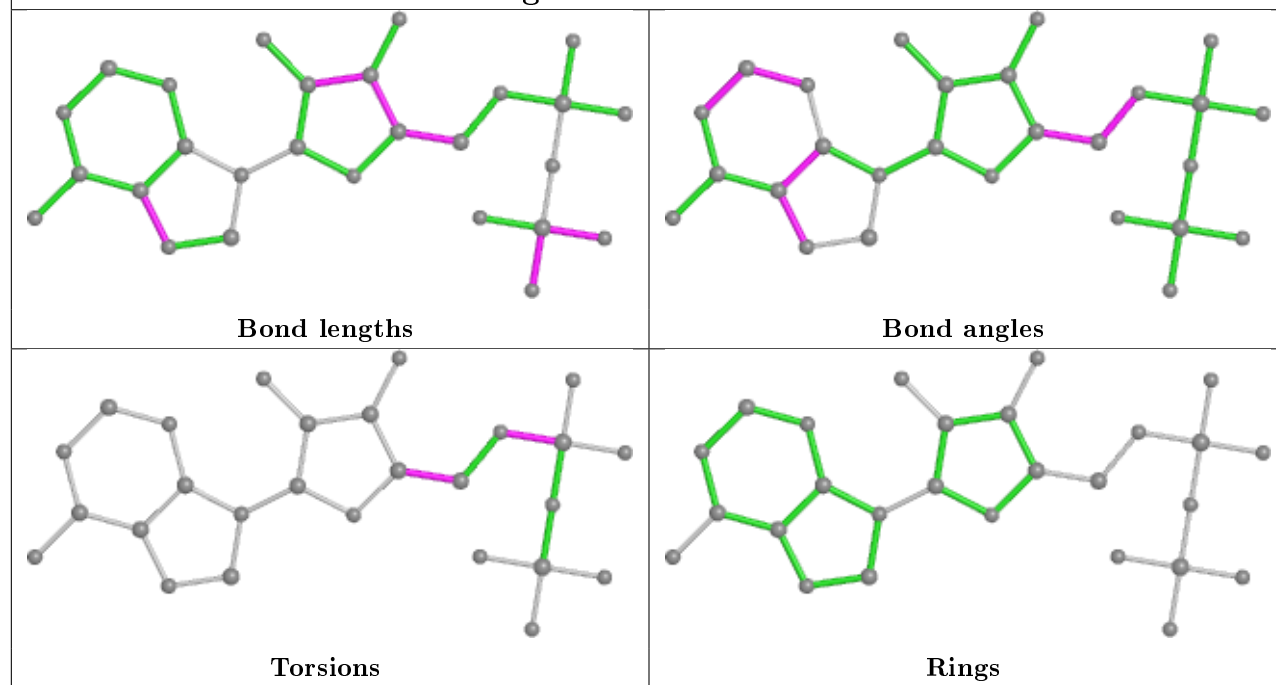
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



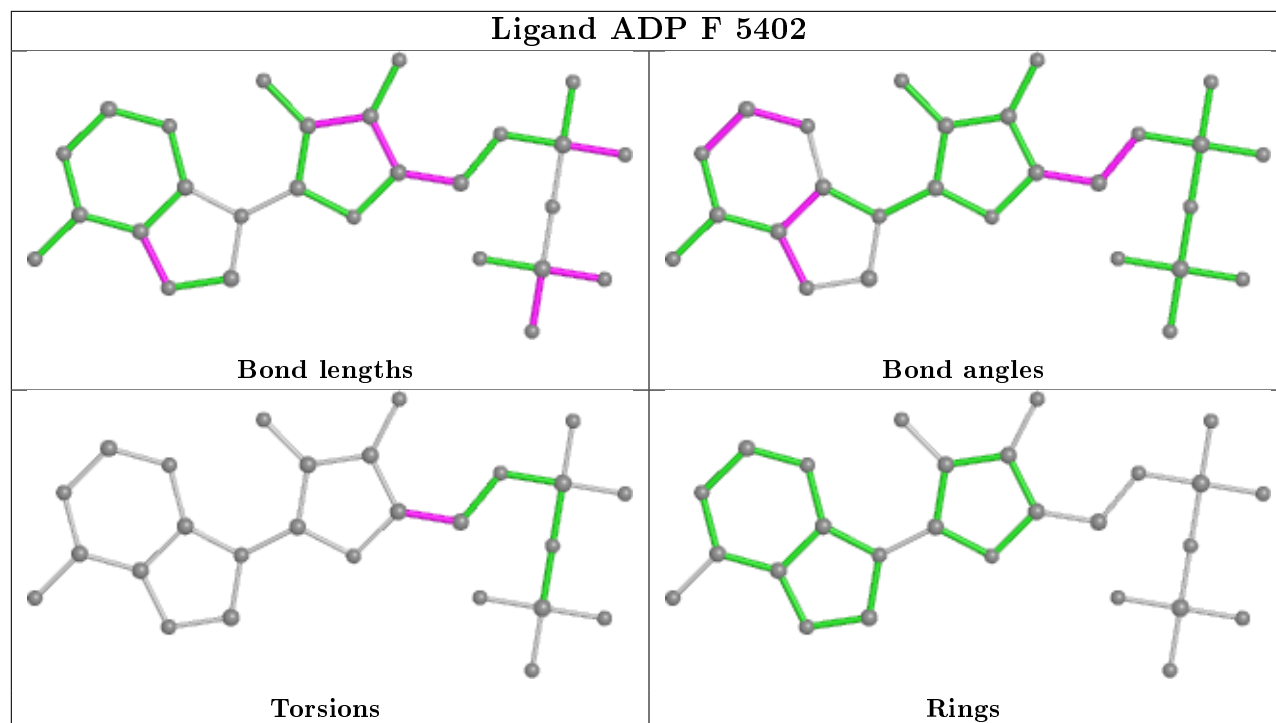
Ligand ADP H 7402



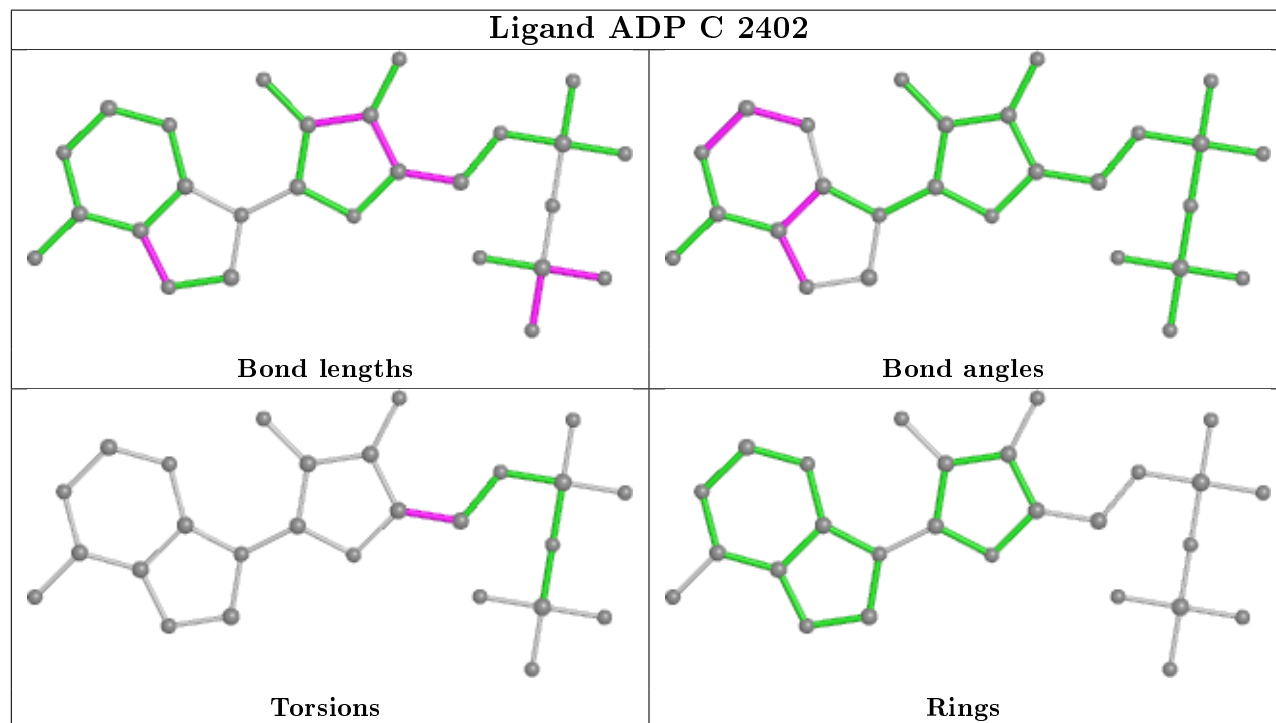
Ligand ADP E 4402

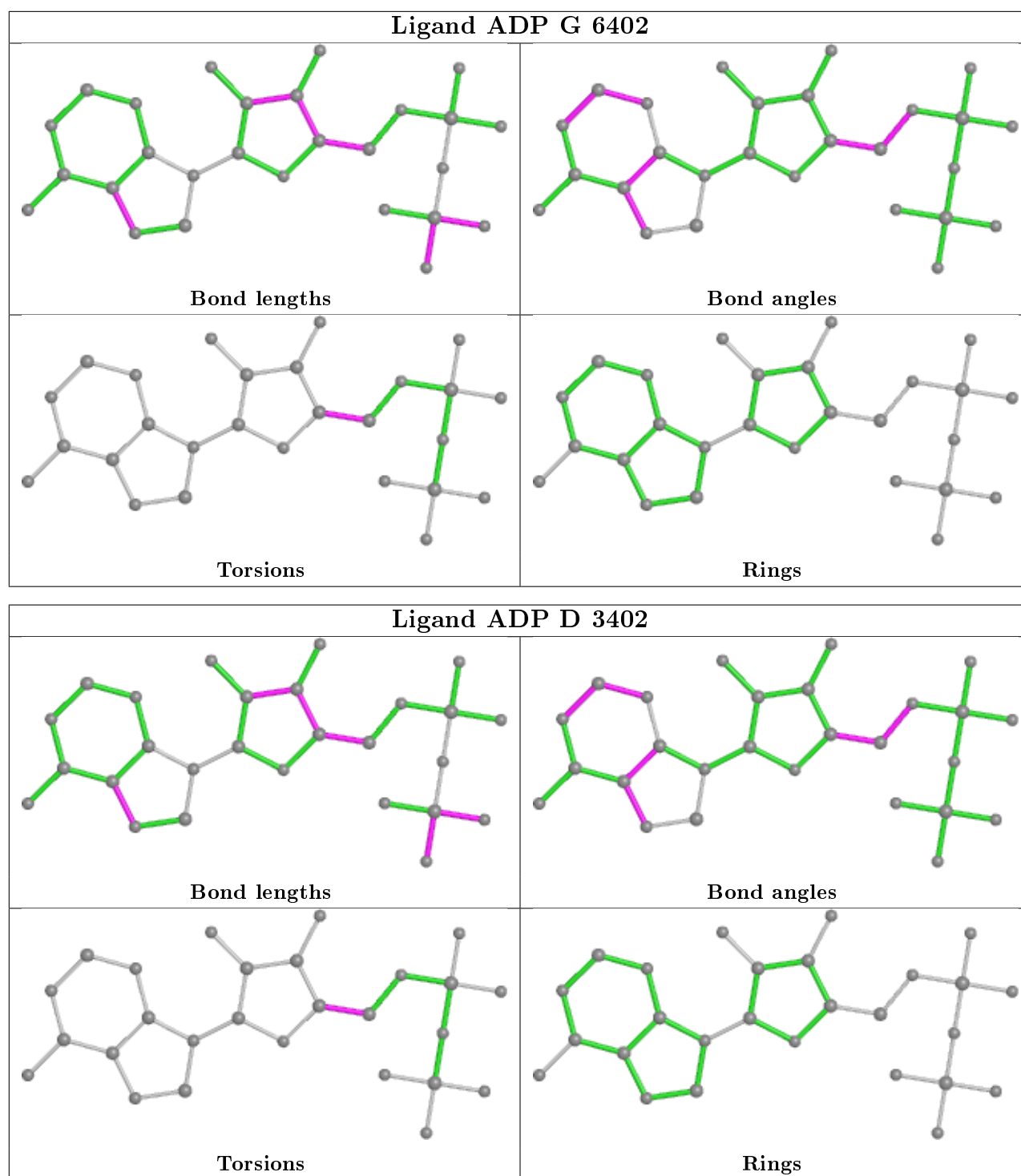


Ligand ADP F 5402



Ligand ADP C 2402





5.7 Other polymers ⓘ

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	312/312 (100%)	-0.16	0 100 100	13, 35, 55, 69	0
1	B	312/312 (100%)	-0.22	1 (0%) 94 93	15, 32, 49, 66	0
1	C	312/312 (100%)	-0.19	3 (0%) 82 77	19, 36, 50, 65	0
1	D	312/312 (100%)	-0.13	7 (2%) 62 52	23, 40, 54, 65	0
1	E	312/312 (100%)	-0.26	0 100 100	9, 31, 47, 61	0
1	F	312/312 (100%)	-0.20	1 (0%) 94 93	7, 32, 49, 65	0
1	G	312/312 (100%)	-0.24	1 (0%) 94 93	20, 37, 53, 63	0
1	H	312/312 (100%)	-0.16	3 (0%) 82 77	24, 39, 52, 61	0
All	All	2496/2496 (100%)	-0.19	16 (0%) 89 86	7, 35, 52, 69	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	196	SER	4.5
1	C	209	ALA	4.3
1	H	310	THR	3.5
1	D	1	MET	3.1
1	D	309	ALA	2.9

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

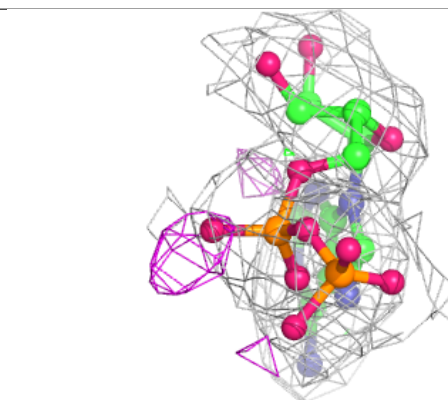
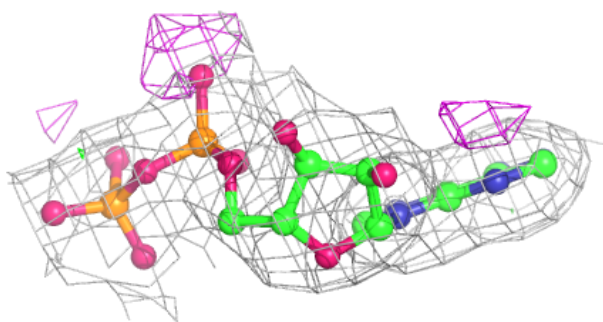
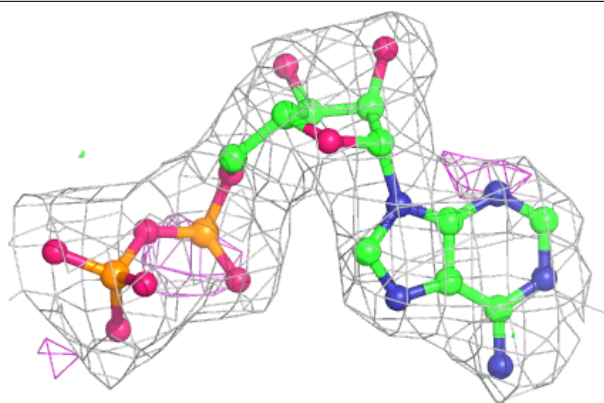
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	ZN	E	4403	1/1	0.94	0.14	59,59,59,59	0
3	PLP	D	3401	15/16	0.95	0.16	40,42,55,56	0
3	PLP	A	401	15/16	0.95	0.16	17,21,44,44	0
4	ADP	E	4402	27/27	0.96	0.18	17,27,32,35	0
4	ADP	D	3402	27/27	0.96	0.17	32,42,50,51	0
2	ZN	B	1403	1/1	0.96	0.17	54,54,54,54	0
3	PLP	C	2401	15/16	0.96	0.20	44,45,55,55	0
4	ADP	H	7402	27/27	0.96	0.15	41,43,53,54	0
2	ZN	G	6403	1/1	0.96	0.12	85,85,85,85	0
4	ADP	A	402	27/27	0.96	0.17	19,26,32,33	0
2	ZN	C	2403	1/1	0.97	0.10	49,49,49,49	0
2	ZN	H	7403	1/1	0.97	0.12	59,59,59,59	0
4	ADP	C	2402	27/27	0.97	0.16	30,33,37,39	0
3	PLP	H	7401	15/16	0.97	0.16	25,26,32,33	0
4	ADP	F	5402	27/27	0.97	0.16	26,31,36,37	0
2	ZN	D	3403	1/1	0.97	0.09	45,45,45,45	0
2	ZN	F	5403	1/1	0.97	0.15	52,52,52,52	0
3	PLP	B	1401	15/16	0.97	0.17	19,24,39,40	0
3	PLP	G	6401	15/16	0.97	0.17	29,32,41,42	0
2	ZN	A	403	1/1	0.97	0.14	48,48,48,48	0
3	PLP	F	5401	15/16	0.97	0.17	14,17,29,31	0
4	ADP	B	1402	27/27	0.98	0.17	17,25,32,32	0
3	PLP	E	4401	15/16	0.98	0.17	11,13,25,26	0
4	ADP	G	6402	27/27	0.98	0.15	30,34,38,39	0

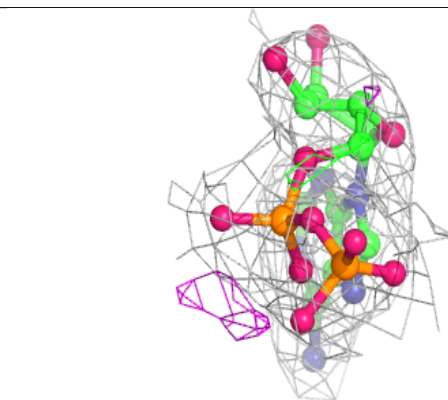
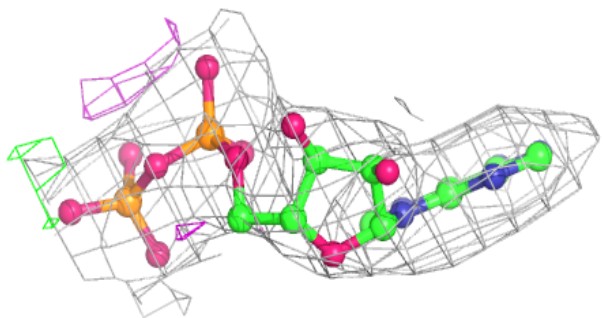
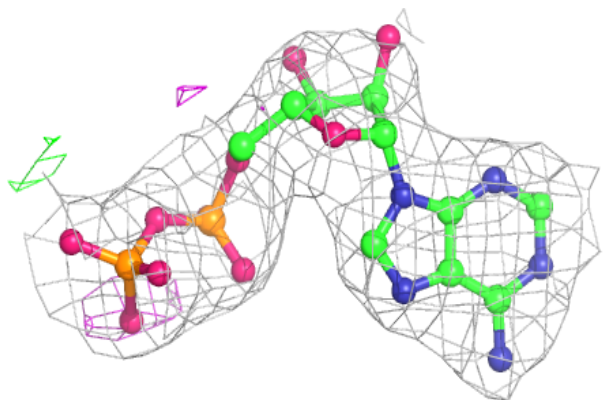
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP E 4402:

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

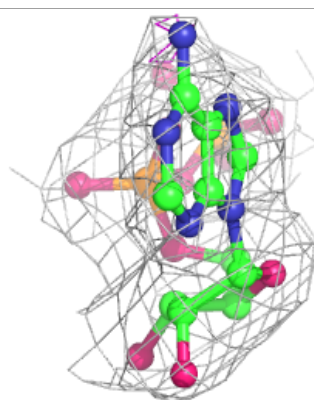
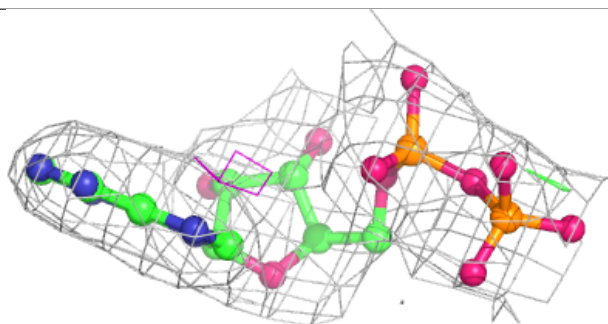
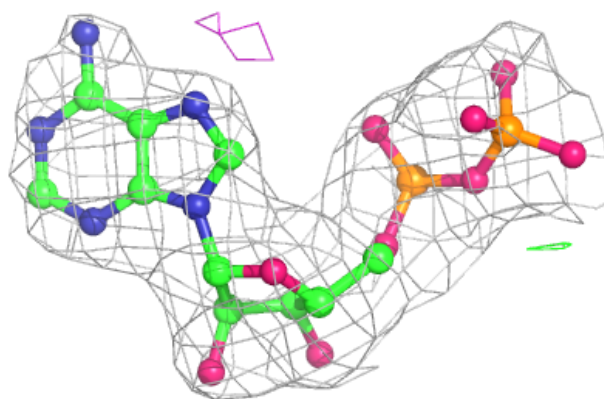
**Electron density around ADP D 3402:**

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

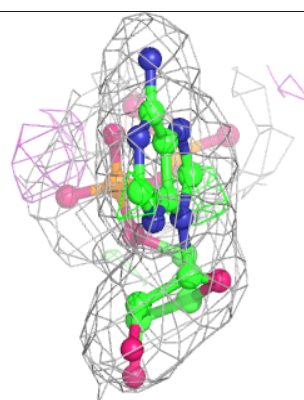
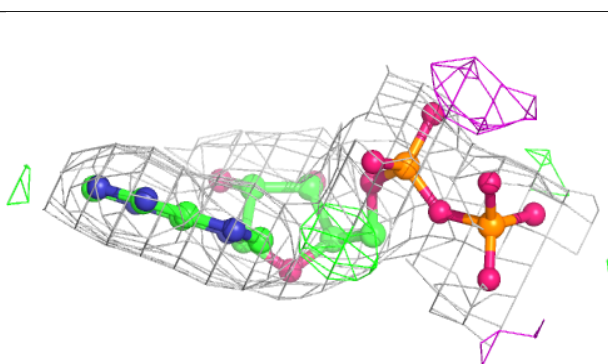
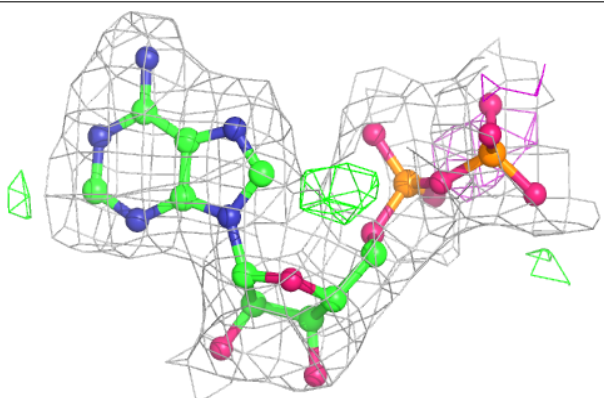


Electron density around ADP H 7402:

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

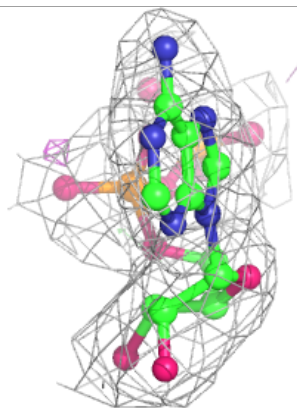
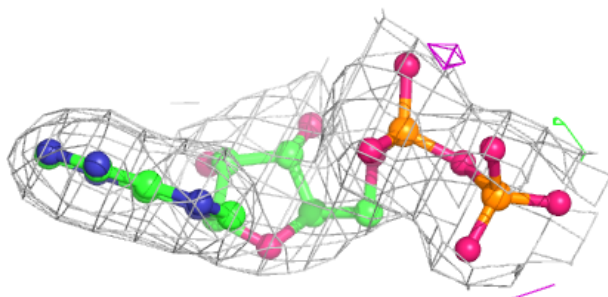
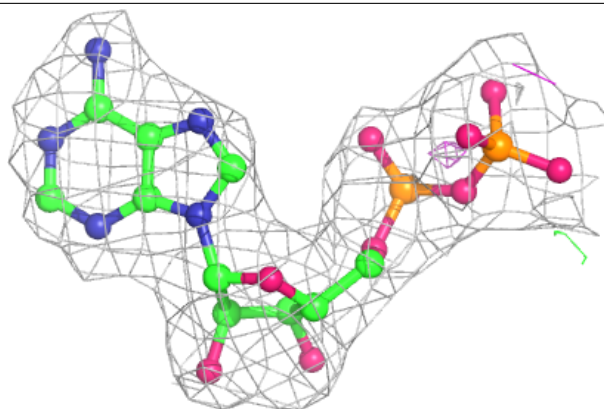
**Electron density around ADP A 402:**

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

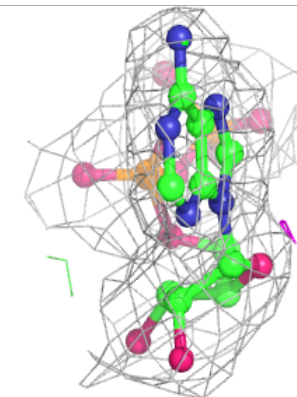
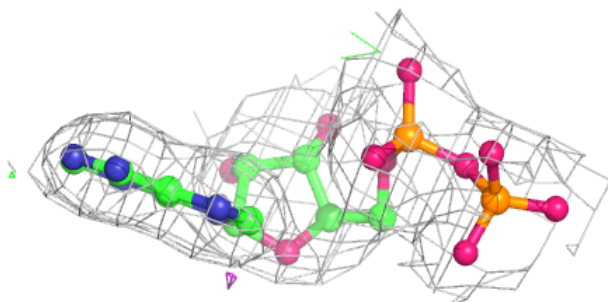
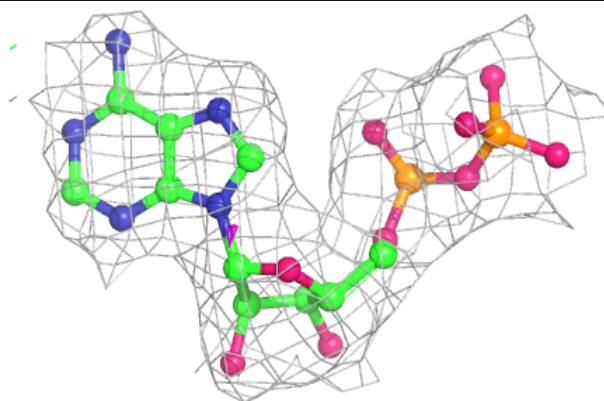


Electron density around ADP C 2402:

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

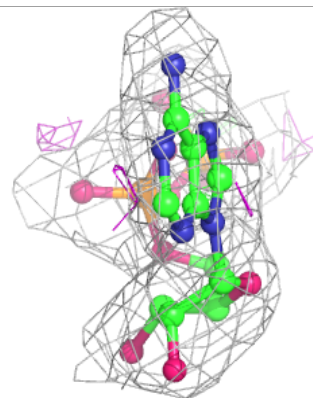
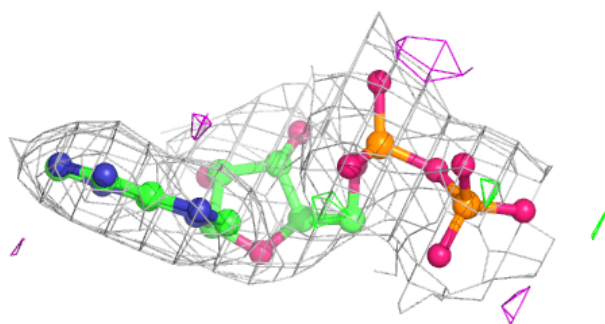
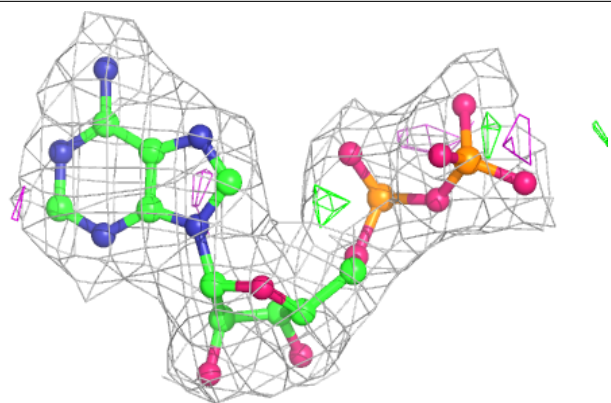
**Electron density around ADP F 5402:**

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

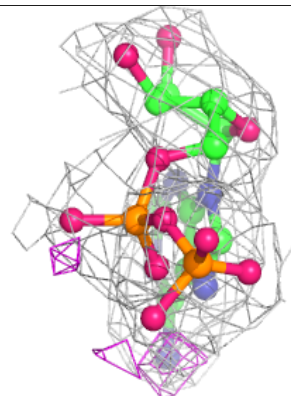
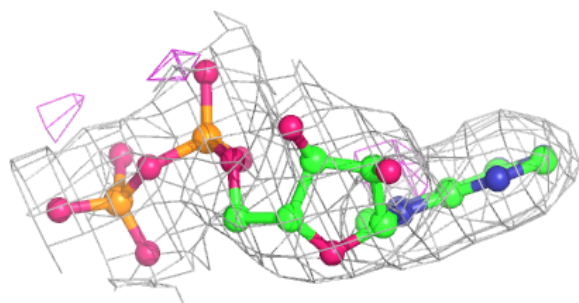
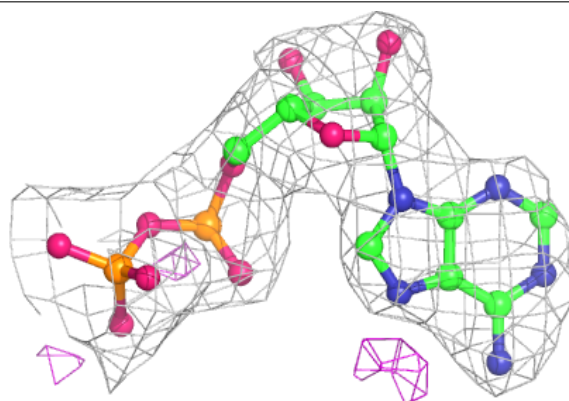


Electron density around ADP B 1402:

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

**Electron density around ADP G 6402:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.