



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 02:24 PM UTC

PDB ID : 7QYS / pdb_00007qys
Title : Crystal structure of RimK from Pseudomonas syringae DC3000
Authors : Thompson, C.M.A.; Little, R.H.; Stevenson, C.E.M.; Lawson, D.M.; Malone, J.G.
Deposited on : 2022-01-29
Resolution : 2.90 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 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

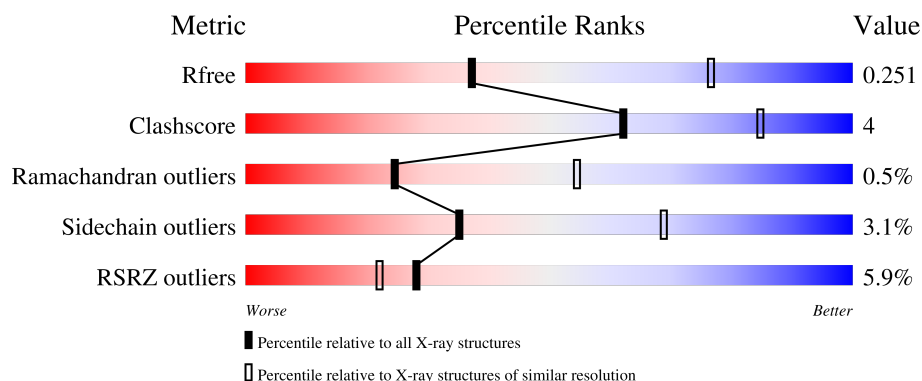
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

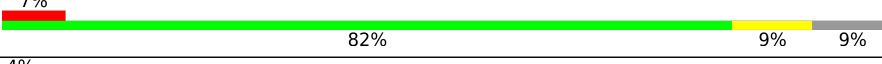
The reported resolution of this entry is 2.90 Å.

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.



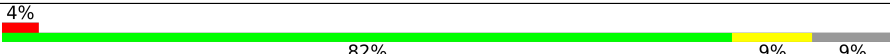
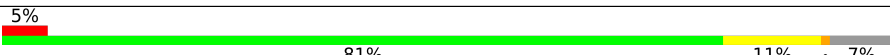
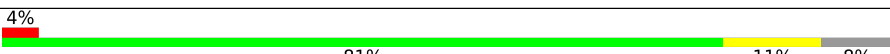
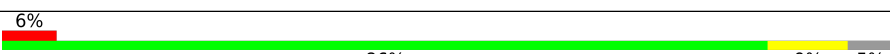
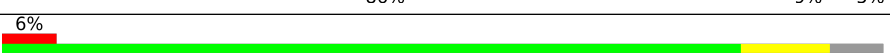
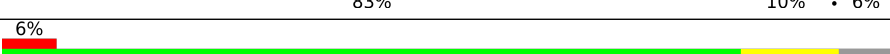
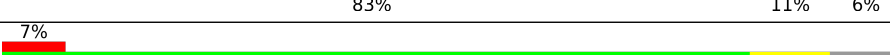
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	309	
1	B	309	
1	C	309	
1	D	309	
1	E	309	

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Mol	Chain	Length	Quality of chain
1	F	309	
1	G	309	
1	H	309	
1	I	309	
1	J	309	
1	K	309	
1	L	309	
1	M	309	
1	N	309	
1	O	309	
1	P	309	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 34293 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 Probable alpha-L-glutamate ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	0	0	0
			2166	1365	383	402	16			
1	B	281	Total	C	N	O	S	0	0	0
			2073	1309	360	388	16			
1	C	282	Total	C	N	O	S	0	0	0
			2108	1332	369	391	16			
1	D	291	Total	C	N	O	S	0	0	0
			2165	1362	385	402	16			
1	E	292	Total	C	N	O	S	0	0	0
			2153	1359	375	403	16			
1	F	284	Total	C	N	O	S	0	0	0
			2121	1338	371	396	16			
1	G	282	Total	C	N	O	S	0	0	0
			2106	1331	366	393	16			
1	H	284	Total	C	N	O	S	0	0	0
			2115	1338	368	393	16			
1	I	282	Total	C	N	O	S	0	0	0
			2080	1315	359	390	16			
1	J	286	Total	C	N	O	S	0	0	0
			2101	1327	361	397	16			
1	K	283	Total	C	N	O	S	0	0	0
			2106	1329	366	395	16			
1	L	294	Total	C	N	O	S	0	0	0
			2178	1374	381	406	17			
1	M	290	Total	C	N	O	S	0	0	0
			2155	1359	380	400	16			
1	N	290	Total	C	N	O	S	0	0	0
			2105	1330	365	394	16			
1	O	290	Total	C	N	O	S	0	0	0
			2147	1355	375	401	16			
1	P	286	Total	C	N	O	S	0	0	0
			2117	1338	368	395	16			

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	302	LEU	-	expression tag	UNP Q88AZ9
A	303	GLU	-	expression tag	UNP Q88AZ9
A	304	HIS	-	expression tag	UNP Q88AZ9
A	305	HIS	-	expression tag	UNP Q88AZ9
A	306	HIS	-	expression tag	UNP Q88AZ9
A	307	HIS	-	expression tag	UNP Q88AZ9
A	308	HIS	-	expression tag	UNP Q88AZ9
A	309	HIS	-	expression tag	UNP Q88AZ9
B	302	LEU	-	expression tag	UNP Q88AZ9
B	303	GLU	-	expression tag	UNP Q88AZ9
B	304	HIS	-	expression tag	UNP Q88AZ9
B	305	HIS	-	expression tag	UNP Q88AZ9
B	306	HIS	-	expression tag	UNP Q88AZ9
B	307	HIS	-	expression tag	UNP Q88AZ9
B	308	HIS	-	expression tag	UNP Q88AZ9
B	309	HIS	-	expression tag	UNP Q88AZ9
C	302	LEU	-	expression tag	UNP Q88AZ9
C	303	GLU	-	expression tag	UNP Q88AZ9
C	304	HIS	-	expression tag	UNP Q88AZ9
C	305	HIS	-	expression tag	UNP Q88AZ9
C	306	HIS	-	expression tag	UNP Q88AZ9
C	307	HIS	-	expression tag	UNP Q88AZ9
C	308	HIS	-	expression tag	UNP Q88AZ9
C	309	HIS	-	expression tag	UNP Q88AZ9
D	302	LEU	-	expression tag	UNP Q88AZ9
D	303	GLU	-	expression tag	UNP Q88AZ9
D	304	HIS	-	expression tag	UNP Q88AZ9
D	305	HIS	-	expression tag	UNP Q88AZ9
D	306	HIS	-	expression tag	UNP Q88AZ9
D	307	HIS	-	expression tag	UNP Q88AZ9
D	308	HIS	-	expression tag	UNP Q88AZ9
D	309	HIS	-	expression tag	UNP Q88AZ9
E	302	LEU	-	expression tag	UNP Q88AZ9
E	303	GLU	-	expression tag	UNP Q88AZ9
E	304	HIS	-	expression tag	UNP Q88AZ9
E	305	HIS	-	expression tag	UNP Q88AZ9
E	306	HIS	-	expression tag	UNP Q88AZ9
E	307	HIS	-	expression tag	UNP Q88AZ9
E	308	HIS	-	expression tag	UNP Q88AZ9
E	309	HIS	-	expression tag	UNP Q88AZ9
F	302	LEU	-	expression tag	UNP Q88AZ9
F	303	GLU	-	expression tag	UNP Q88AZ9

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Chain	Residue	Modelled	Actual	Comment	Reference
F	304	HIS	-	expression tag	UNP Q88AZ9
F	305	HIS	-	expression tag	UNP Q88AZ9
F	306	HIS	-	expression tag	UNP Q88AZ9
F	307	HIS	-	expression tag	UNP Q88AZ9
F	308	HIS	-	expression tag	UNP Q88AZ9
F	309	HIS	-	expression tag	UNP Q88AZ9
G	302	LEU	-	expression tag	UNP Q88AZ9
G	303	GLU	-	expression tag	UNP Q88AZ9
G	304	HIS	-	expression tag	UNP Q88AZ9
G	305	HIS	-	expression tag	UNP Q88AZ9
G	306	HIS	-	expression tag	UNP Q88AZ9
G	307	HIS	-	expression tag	UNP Q88AZ9
G	308	HIS	-	expression tag	UNP Q88AZ9
G	309	HIS	-	expression tag	UNP Q88AZ9
H	302	LEU	-	expression tag	UNP Q88AZ9
H	303	GLU	-	expression tag	UNP Q88AZ9
H	304	HIS	-	expression tag	UNP Q88AZ9
H	305	HIS	-	expression tag	UNP Q88AZ9
H	306	HIS	-	expression tag	UNP Q88AZ9
H	307	HIS	-	expression tag	UNP Q88AZ9
H	308	HIS	-	expression tag	UNP Q88AZ9
H	309	HIS	-	expression tag	UNP Q88AZ9
I	302	LEU	-	expression tag	UNP Q88AZ9
I	303	GLU	-	expression tag	UNP Q88AZ9
I	304	HIS	-	expression tag	UNP Q88AZ9
I	305	HIS	-	expression tag	UNP Q88AZ9
I	306	HIS	-	expression tag	UNP Q88AZ9
I	307	HIS	-	expression tag	UNP Q88AZ9
I	308	HIS	-	expression tag	UNP Q88AZ9
I	309	HIS	-	expression tag	UNP Q88AZ9
J	302	LEU	-	expression tag	UNP Q88AZ9
J	303	GLU	-	expression tag	UNP Q88AZ9
J	304	HIS	-	expression tag	UNP Q88AZ9
J	305	HIS	-	expression tag	UNP Q88AZ9
J	306	HIS	-	expression tag	UNP Q88AZ9
J	307	HIS	-	expression tag	UNP Q88AZ9
J	308	HIS	-	expression tag	UNP Q88AZ9
J	309	HIS	-	expression tag	UNP Q88AZ9
K	302	LEU	-	expression tag	UNP Q88AZ9
K	303	GLU	-	expression tag	UNP Q88AZ9
K	304	HIS	-	expression tag	UNP Q88AZ9
K	305	HIS	-	expression tag	UNP Q88AZ9

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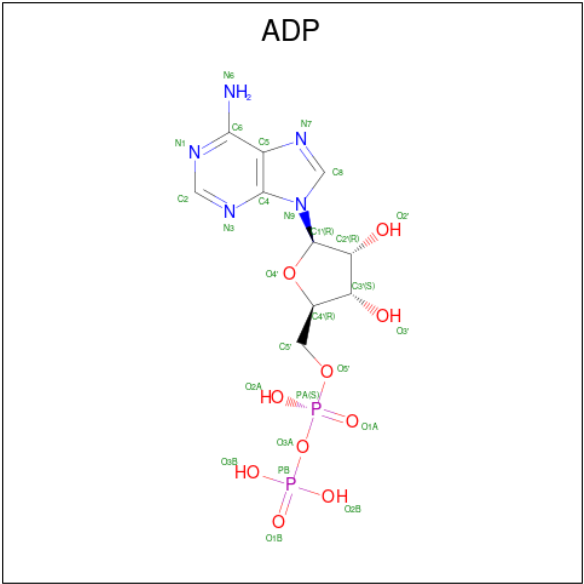
Chain	Residue	Modelled	Actual	Comment	Reference
K	306	HIS	-	expression tag	UNP Q88AZ9
K	307	HIS	-	expression tag	UNP Q88AZ9
K	308	HIS	-	expression tag	UNP Q88AZ9
K	309	HIS	-	expression tag	UNP Q88AZ9
L	302	LEU	-	expression tag	UNP Q88AZ9
L	303	GLU	-	expression tag	UNP Q88AZ9
L	304	HIS	-	expression tag	UNP Q88AZ9
L	305	HIS	-	expression tag	UNP Q88AZ9
L	306	HIS	-	expression tag	UNP Q88AZ9
L	307	HIS	-	expression tag	UNP Q88AZ9
L	308	HIS	-	expression tag	UNP Q88AZ9
L	309	HIS	-	expression tag	UNP Q88AZ9
M	302	LEU	-	expression tag	UNP Q88AZ9
M	303	GLU	-	expression tag	UNP Q88AZ9
M	304	HIS	-	expression tag	UNP Q88AZ9
M	305	HIS	-	expression tag	UNP Q88AZ9
M	306	HIS	-	expression tag	UNP Q88AZ9
M	307	HIS	-	expression tag	UNP Q88AZ9
M	308	HIS	-	expression tag	UNP Q88AZ9
M	309	HIS	-	expression tag	UNP Q88AZ9
N	302	LEU	-	expression tag	UNP Q88AZ9
N	303	GLU	-	expression tag	UNP Q88AZ9
N	304	HIS	-	expression tag	UNP Q88AZ9
N	305	HIS	-	expression tag	UNP Q88AZ9
N	306	HIS	-	expression tag	UNP Q88AZ9
N	307	HIS	-	expression tag	UNP Q88AZ9
N	308	HIS	-	expression tag	UNP Q88AZ9
N	309	HIS	-	expression tag	UNP Q88AZ9
O	302	LEU	-	expression tag	UNP Q88AZ9
O	303	GLU	-	expression tag	UNP Q88AZ9
O	304	HIS	-	expression tag	UNP Q88AZ9
O	305	HIS	-	expression tag	UNP Q88AZ9
O	306	HIS	-	expression tag	UNP Q88AZ9
O	307	HIS	-	expression tag	UNP Q88AZ9
O	308	HIS	-	expression tag	UNP Q88AZ9
O	309	HIS	-	expression tag	UNP Q88AZ9
P	302	LEU	-	expression tag	UNP Q88AZ9
P	303	GLU	-	expression tag	UNP Q88AZ9
P	304	HIS	-	expression tag	UNP Q88AZ9
P	305	HIS	-	expression tag	UNP Q88AZ9
P	306	HIS	-	expression tag	UNP Q88AZ9
P	307	HIS	-	expression tag	UNP Q88AZ9

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Chain	Residue	Modelled	Actual	Comment	Reference
P	308	HIS	-	expression tag	UNP Q88AZ9
P	309	HIS	-	expression tag	UNP Q88AZ9

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



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

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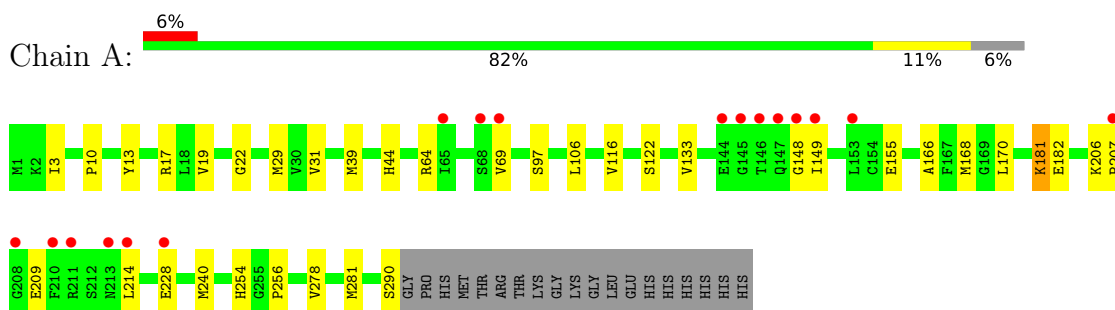
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	O	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

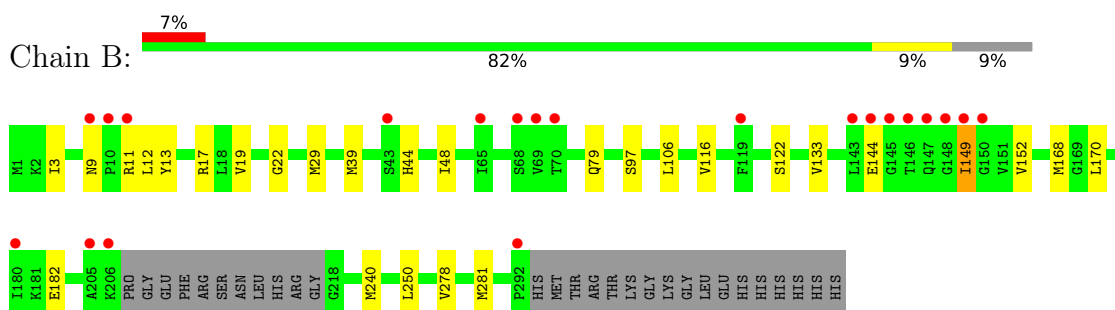
3 Residue-property plots [i](#)

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.

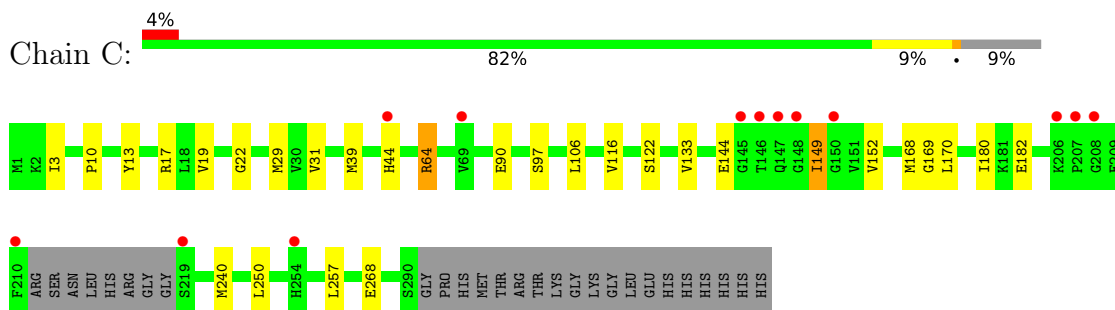
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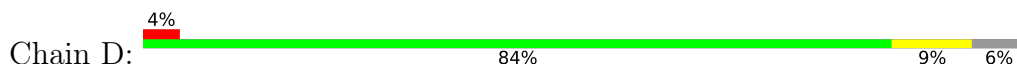
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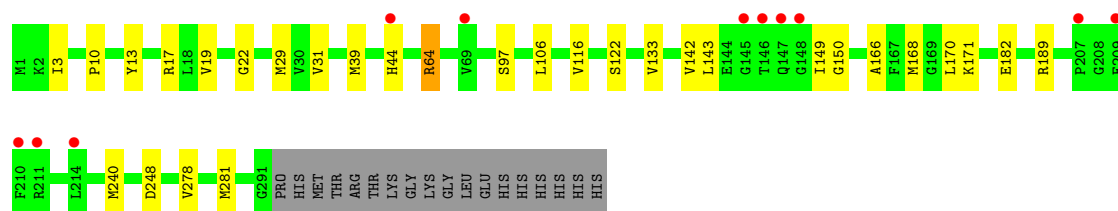


- Molecule 1: Probable alpha-L-glutamate ligase

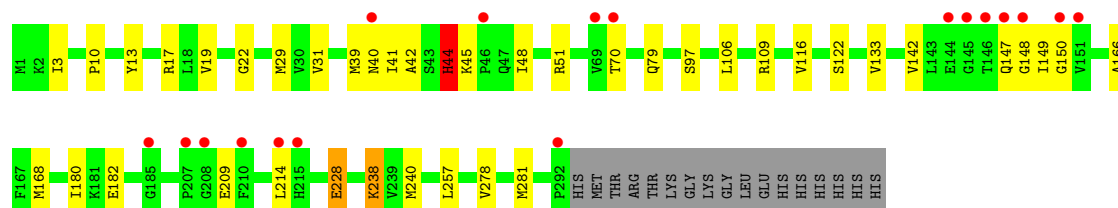
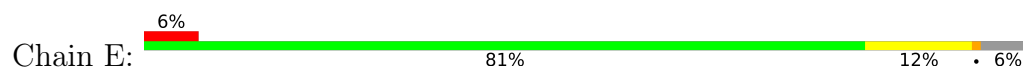


- Molecule 1: Probable alpha-L-glutamate ligase

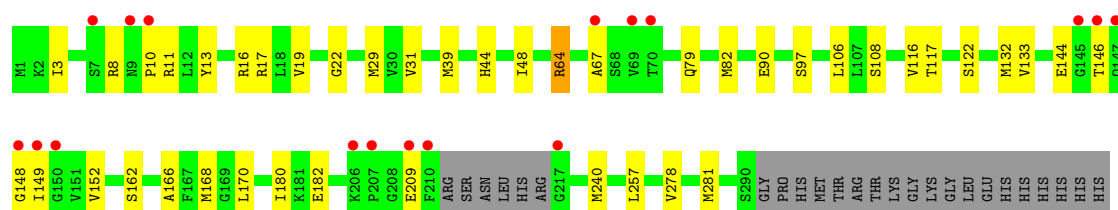
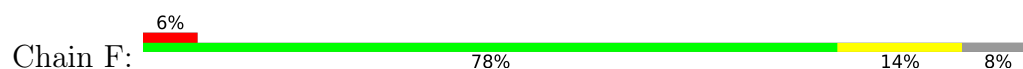




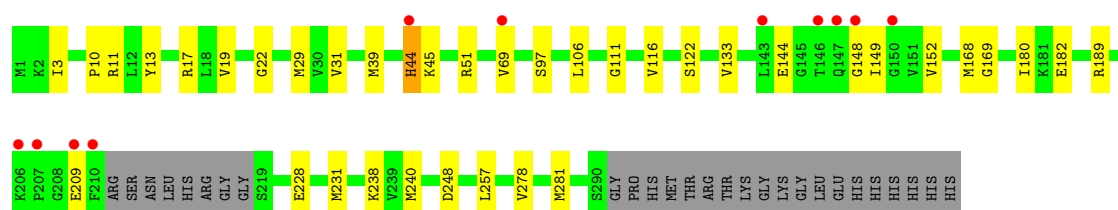
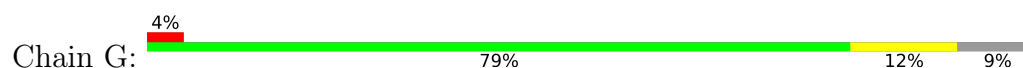
- Molecule 1: Probable alpha-L-glutamate ligase



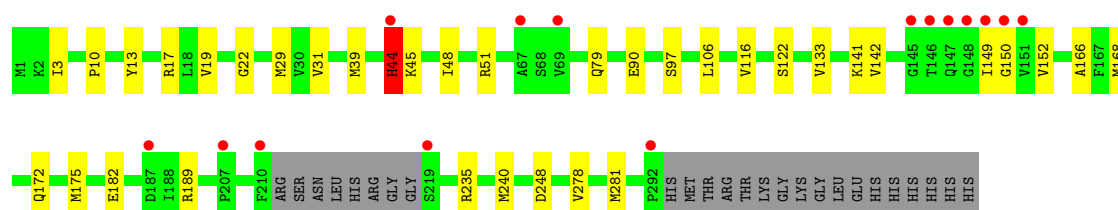
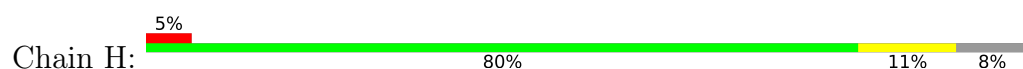
- Molecule 1: Probable alpha-L-glutamate ligase



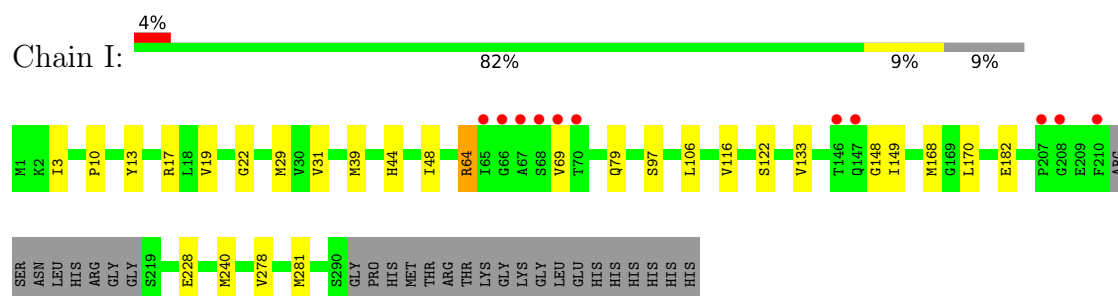
- Molecule 1: Probable alpha-L-glutamate ligase



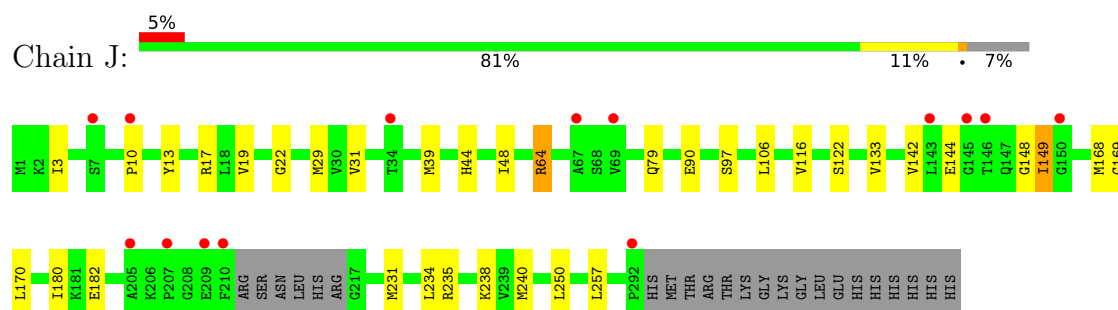
- Molecule 1: Probable alpha-L-glutamate ligase



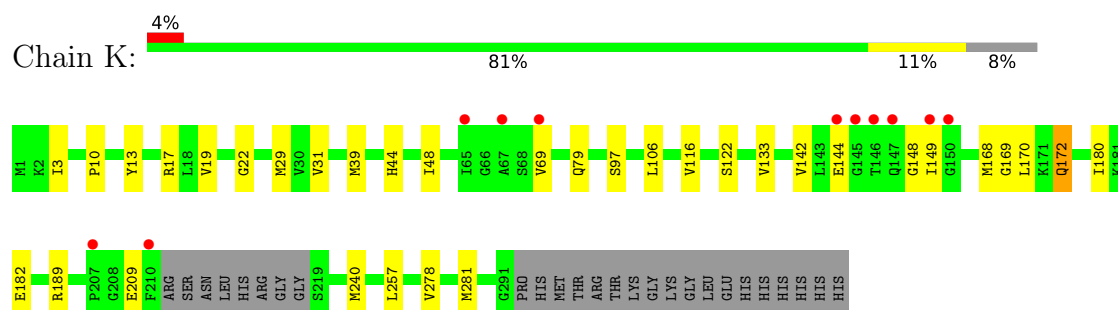
- Molecule 1: Probable alpha-L-glutamate ligase



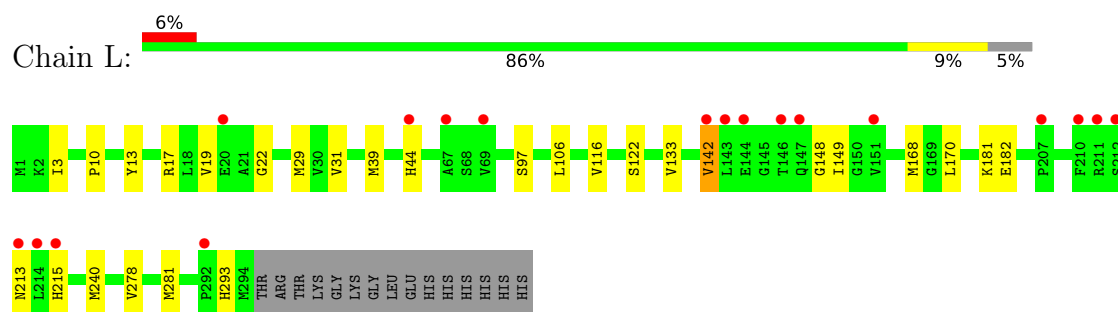
- Molecule 1: Probable alpha-L-glutamate ligase



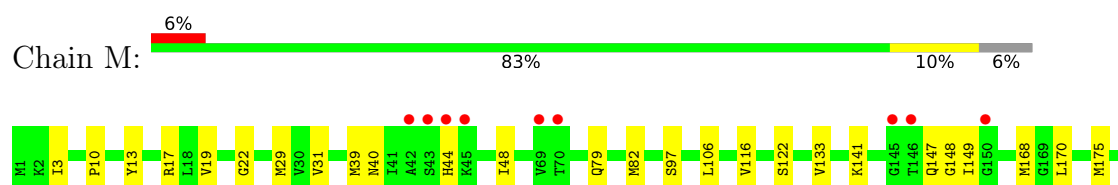
- Molecule 1: Probable alpha-L-glutamate ligase



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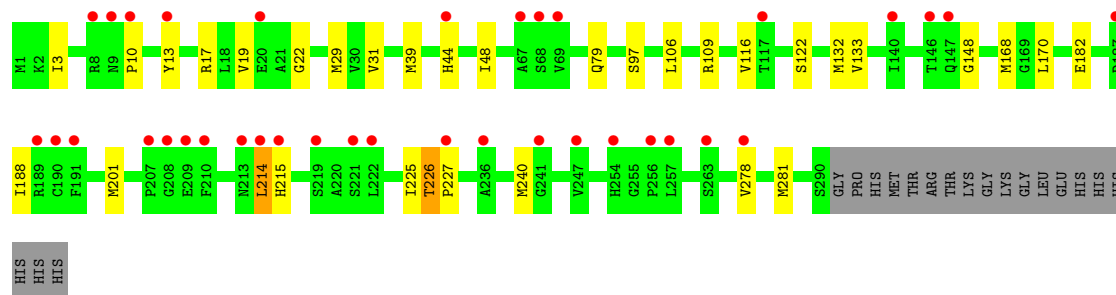
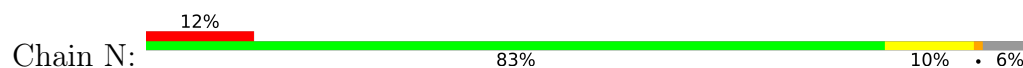


- Molecule 1: Probable alpha-L-glutamate ligase

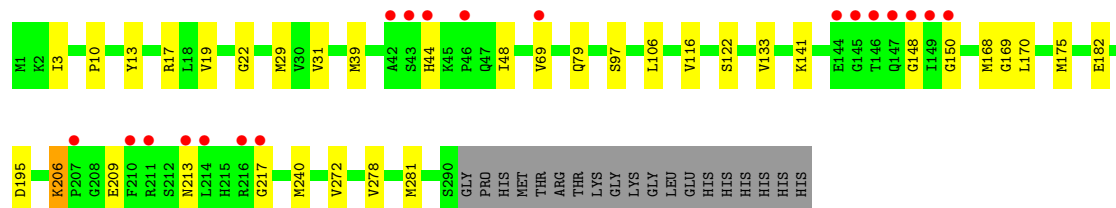
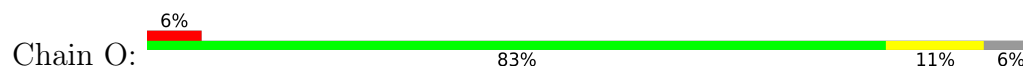




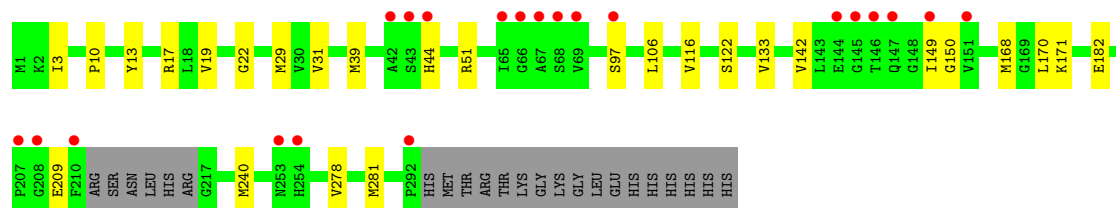
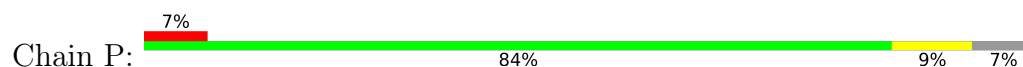
- Molecule 1: Probable alpha-L-glutamate ligase



- Molecule 1: Probable alpha-L-glutamate ligase



- Molecule 1: Probable alpha-L-glutamate ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	95.91Å 96.09Å 156.99Å 88.94° 84.37° 89.97°	Depositor
Resolution (Å)	49.80 – 2.90 49.80 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.80-2.90) 98.9 (49.80-2.90)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.237 , 0.248 0.240 , 0.251	Depositor DCC
R_{free} test set	5894 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	56.3	Xtriage
Anisotropy	0.559	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.104 for -h,k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	34293	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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: ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.02	0/2197	1.49	3/2968 (0.1%)
1	B	1.05	0/2102	1.49	0/2848
1	C	1.02	0/2138	1.48	3/2891 (0.1%)
1	D	1.02	0/2196	1.49	1/2969 (0.0%)
1	E	1.04	1/2185 (0.0%)	1.52	6/2959 (0.2%)
1	F	1.01	0/2151	1.50	5/2907 (0.2%)
1	G	1.02	0/2136	1.47	2/2889 (0.1%)
1	H	1.02	0/2146	1.48	0/2903
1	I	1.02	0/2110	1.49	5/2857 (0.2%)
1	J	1.02	0/2131	1.50	5/2887 (0.2%)
1	K	1.01	0/2136	1.48	3/2889 (0.1%)
1	L	1.02	0/2211	1.49	2/2991 (0.1%)
1	M	1.01	0/2186	1.48	2/2955 (0.1%)
1	N	1.04	0/2136	1.50	3/2897 (0.1%)
1	O	1.02	0/2178	1.47	3/2946 (0.1%)
1	P	1.02	0/2148	1.47	0/2906
All	All	1.02	1/34487 (0.0%)	1.49	43/46662 (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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	44	HIS	C-O	-6.62	1.15	1.24

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	45	LYS	CB-CA-C	9.84	121.07	109.85
1	I	64	ARG	NE-CZ-NH2	8.11	126.50	119.20
1	C	64	ARG	NE-CZ-NH2	7.92	126.33	119.20
1	J	64	ARG	NE-CZ-NH2	7.80	126.22	119.20
1	F	64	ARG	NE-CZ-NH2	7.65	126.08	119.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	44	HIS	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	2166	0	2212	28	0
1	B	2073	0	2084	18	0
1	C	2108	0	2148	19	1
1	D	2165	0	2197	21	0
1	E	2153	0	2176	21	1
1	F	2121	0	2161	36	0
1	G	2106	0	2141	23	0
1	H	2115	0	2151	27	0
1	I	2080	0	2085	19	0
1	J	2101	0	2113	25	0
1	K	2106	0	2131	22	0
1	L	2178	0	2200	15	0
1	M	2155	0	2195	19	0
1	N	2105	0	2095	23	0
1	O	2147	0	2179	22	0
1	P	2117	0	2145	17	0
2	A	27	0	12	0	0
2	B	27	0	12	1	0
2	C	27	0	12	1	0
2	D	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	27	0	12	0	0
2	G	27	0	12	0	0
2	H	27	0	12	0	0
2	J	27	0	12	1	0
2	K	27	0	12	0	0
2	M	27	0	12	0	0
2	O	27	0	12	0	0
All	All	34293	0	34545	285	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 4.

The worst 5 of 285 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:I:228:GLU:HG2	1:O:272:VAL:HG21	1.47	0.92
1:N:226:THR:HG22	1:N:227:PRO:HD2	1.55	0.89
1:A:181:LYS:HB2	1:F:11:ARG:CB	2.02	0.88
1:J:3:ILE:HD12	1:J:29:MET:HE1	1.59	0.85
1:B:3:ILE:HD12	1:B:29:MET:HE1	1.59	0.84

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:C:268:GLU:OE2	1:E:228:GLU:OE1[1_545]	1.75	0.45

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	288/309 (93%)	274 (95%)	12 (4%)	2 (1%)	18	48
1	B	277/309 (90%)	266 (96%)	10 (4%)	1 (0%)	30	59
1	C	278/309 (90%)	266 (96%)	11 (4%)	1 (0%)	30	59
1	D	289/309 (94%)	274 (95%)	14 (5%)	1 (0%)	36	65
1	E	290/309 (94%)	276 (95%)	13 (4%)	1 (0%)	36	65
1	F	280/309 (91%)	267 (95%)	12 (4%)	1 (0%)	30	59
1	G	278/309 (90%)	266 (96%)	10 (4%)	2 (1%)	18	48
1	H	280/309 (91%)	268 (96%)	11 (4%)	1 (0%)	30	59
1	I	278/309 (90%)	266 (96%)	10 (4%)	2 (1%)	18	48
1	J	282/309 (91%)	271 (96%)	10 (4%)	1 (0%)	30	59
1	K	279/309 (90%)	267 (96%)	10 (4%)	2 (1%)	18	48
1	L	292/309 (94%)	276 (94%)	14 (5%)	2 (1%)	18	48
1	M	288/309 (93%)	275 (96%)	12 (4%)	1 (0%)	36	65
1	N	288/309 (93%)	273 (95%)	14 (5%)	1 (0%)	36	65
1	O	288/309 (93%)	274 (95%)	12 (4%)	2 (1%)	18	48
1	P	282/309 (91%)	268 (95%)	13 (5%)	1 (0%)	30	59
All	All	4537/4944 (92%)	4327 (95%)	188 (4%)	22 (0%)	24	54

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	HIS
1	B	44	HIS
1	C	44	HIS
1	D	44	HIS
1	F	44	HIS

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	229/254 (90%)	222 (97%)	7 (3%)	35	69
1	B	215/254 (85%)	209 (97%)	6 (3%)	38	72
1	C	223/254 (88%)	216 (97%)	7 (3%)	35	69
1	D	227/254 (89%)	221 (97%)	6 (3%)	40	73
1	E	226/254 (89%)	217 (96%)	9 (4%)	28	62
1	F	225/254 (89%)	217 (96%)	8 (4%)	31	65
1	G	223/254 (88%)	216 (97%)	7 (3%)	35	69
1	H	223/254 (88%)	215 (96%)	8 (4%)	31	65
1	I	216/254 (85%)	211 (98%)	5 (2%)	44	76
1	J	220/254 (87%)	213 (97%)	7 (3%)	34	68
1	K	222/254 (87%)	216 (97%)	6 (3%)	39	73
1	L	228/254 (90%)	220 (96%)	8 (4%)	32	66
1	M	227/254 (89%)	219 (96%)	8 (4%)	32	66
1	N	215/254 (85%)	209 (97%)	6 (3%)	38	72
1	O	226/254 (89%)	219 (97%)	7 (3%)	35	69
1	P	222/254 (87%)	215 (97%)	7 (3%)	34	68
All	All	3567/4064 (88%)	3455 (97%)	112 (3%)	35	69

5 of 112 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	235	ARG
1	P	182	GLU
1	K	39	MET
1	P	171	LYS
1	O	39	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	131	GLN
1	O	105	GLN
1	K	134	ASN
1	M	134	ASN
1	O	134	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 ⓘ

11 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ADP	B	401	-	28,29,29	0.51	0	43,45,45	0.40	0
2	ADP	J	401	-	28,29,29	0.49	0	43,45,45	0.46	0
2	ADP	G	401	-	28,29,29	0.51	0	43,45,45	0.47	0
2	ADP	K	401	-	28,29,29	0.52	0	43,45,45	0.46	0
2	ADP	A	401	-	28,29,29	0.46	0	43,45,45	0.54	0
2	ADP	D	401	-	28,29,29	0.51	0	43,45,45	0.46	0
2	ADP	E	401	-	28,29,29	0.51	0	43,45,45	0.48	0
2	ADP	M	401	-	28,29,29	0.48	0	43,45,45	0.51	0
2	ADP	H	401	-	28,29,29	0.53	0	43,45,45	0.45	0
2	ADP	C	401	-	28,29,29	0.53	0	43,45,45	0.54	0
2	ADP	O	401	-	28,29,29	0.53	0	43,45,45	0.46	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	ADP	B	401	-	-	1/16/32/32	0/3/3/3
2	ADP	J	401	-	-	1/16/32/32	0/3/3/3
2	ADP	G	401	-	-	2/16/32/32	0/3/3/3
2	ADP	K	401	-	-	5/16/32/32	0/3/3/3
2	ADP	A	401	-	-	6/16/32/32	0/3/3/3
2	ADP	D	401	-	-	2/16/32/32	0/3/3/3
2	ADP	E	401	-	-	3/16/32/32	0/3/3/3
2	ADP	M	401	-	-	4/16/32/32	0/3/3/3
2	ADP	H	401	-	-	8/16/32/32	0/3/3/3
2	ADP	C	401	-	-	4/16/32/32	0/3/3/3
2	ADP	O	401	-	-	2/16/32/32	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	ADP	C5'-O5'-PA-O1A
2	A	401	ADP	C5'-O5'-PA-O2A
2	A	401	ADP	C5'-O5'-PA-O3A
2	C	401	ADP	O4'-C4'-C5'-O5'
2	D	401	ADP	C5'-O5'-PA-O1A

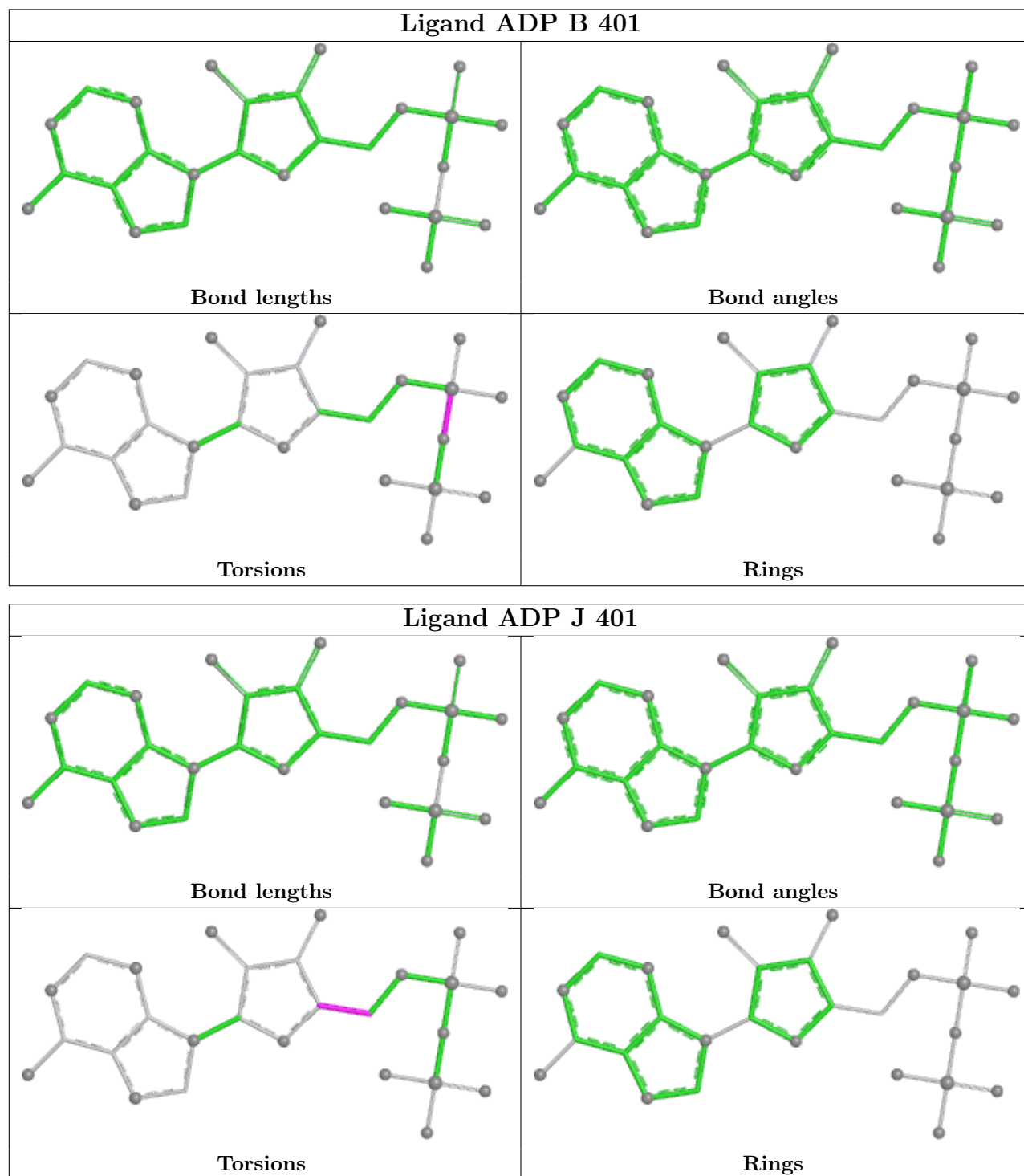
There are no ring outliers.

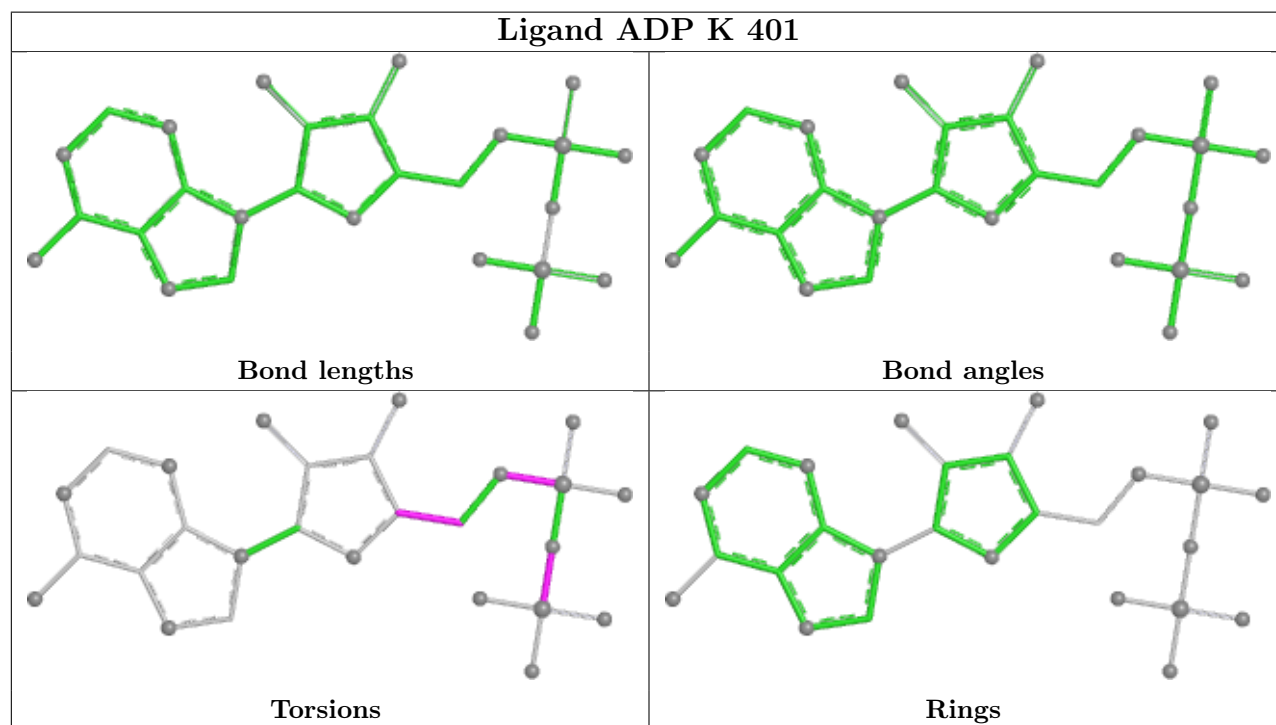
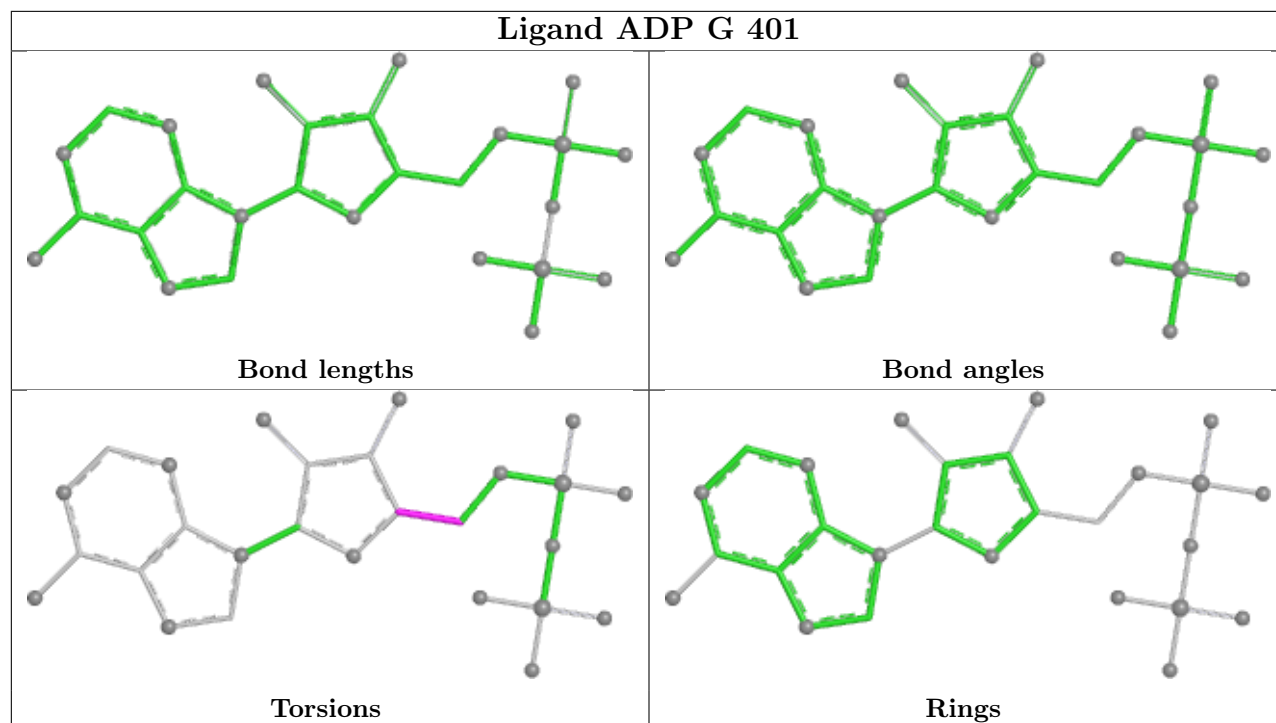
3 monomers are involved in 3 short contacts:

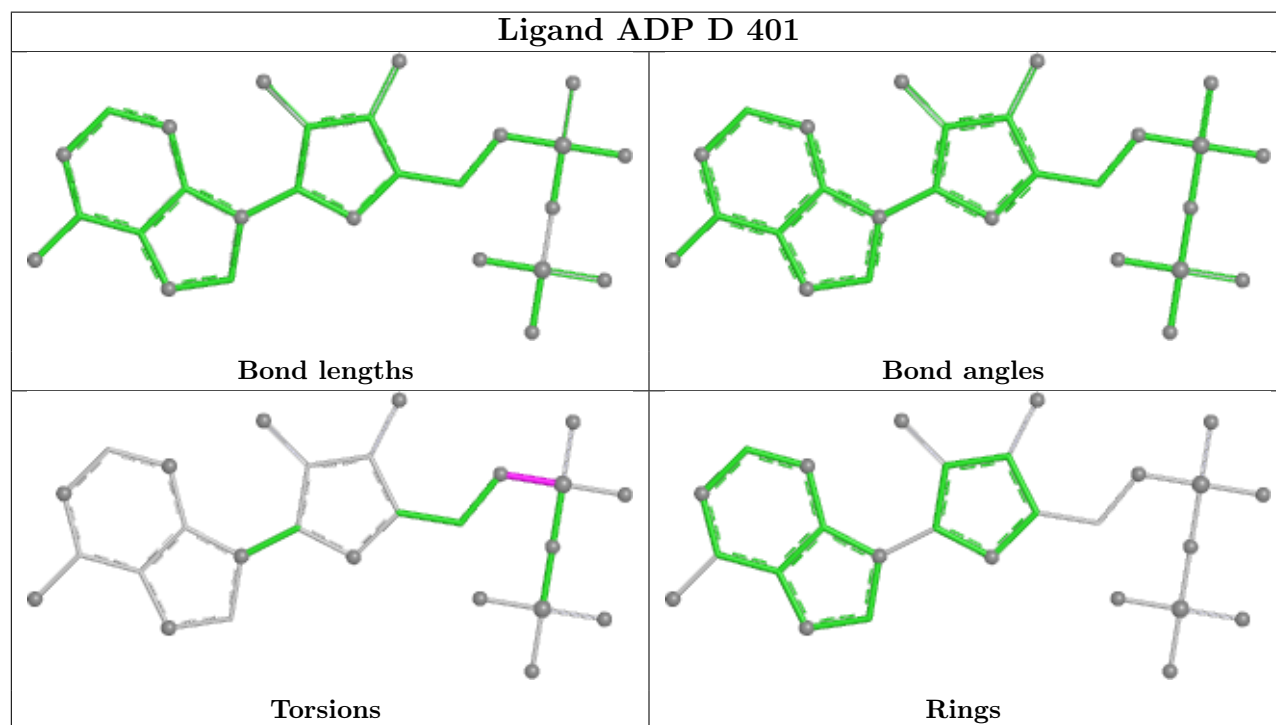
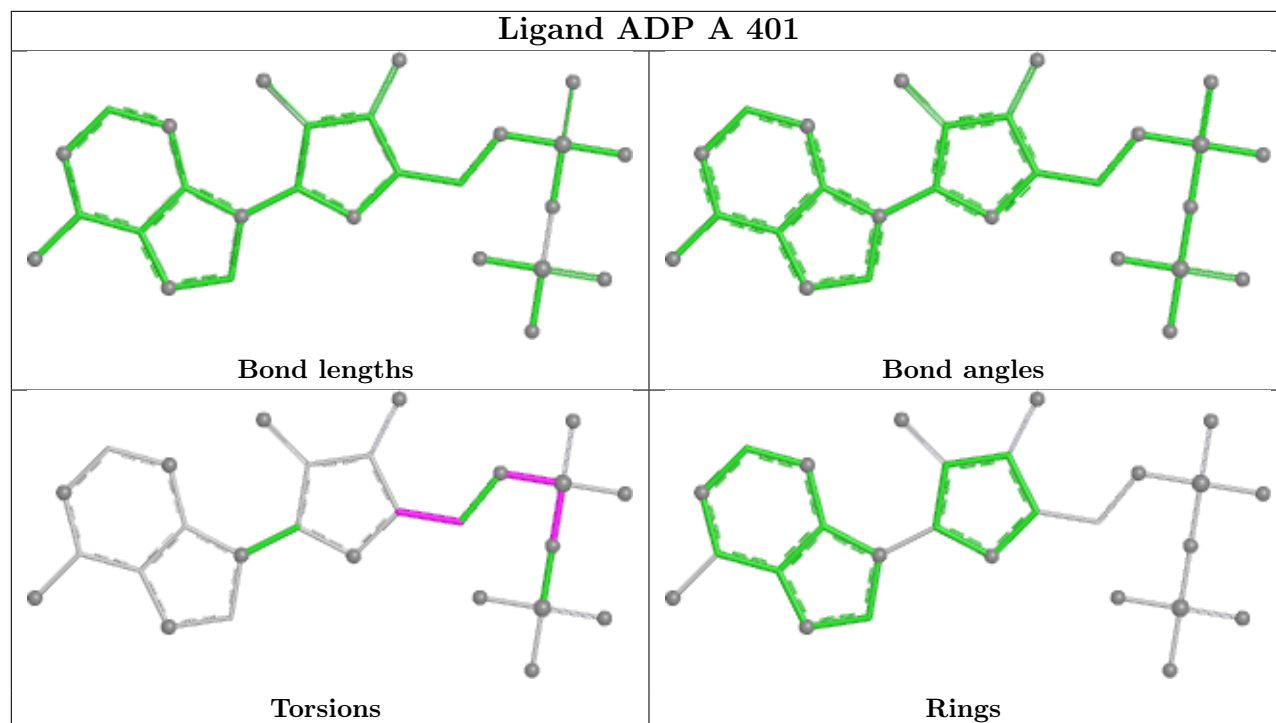
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	ADP	1	0
2	J	401	ADP	1	0
2	C	401	ADP	1	0

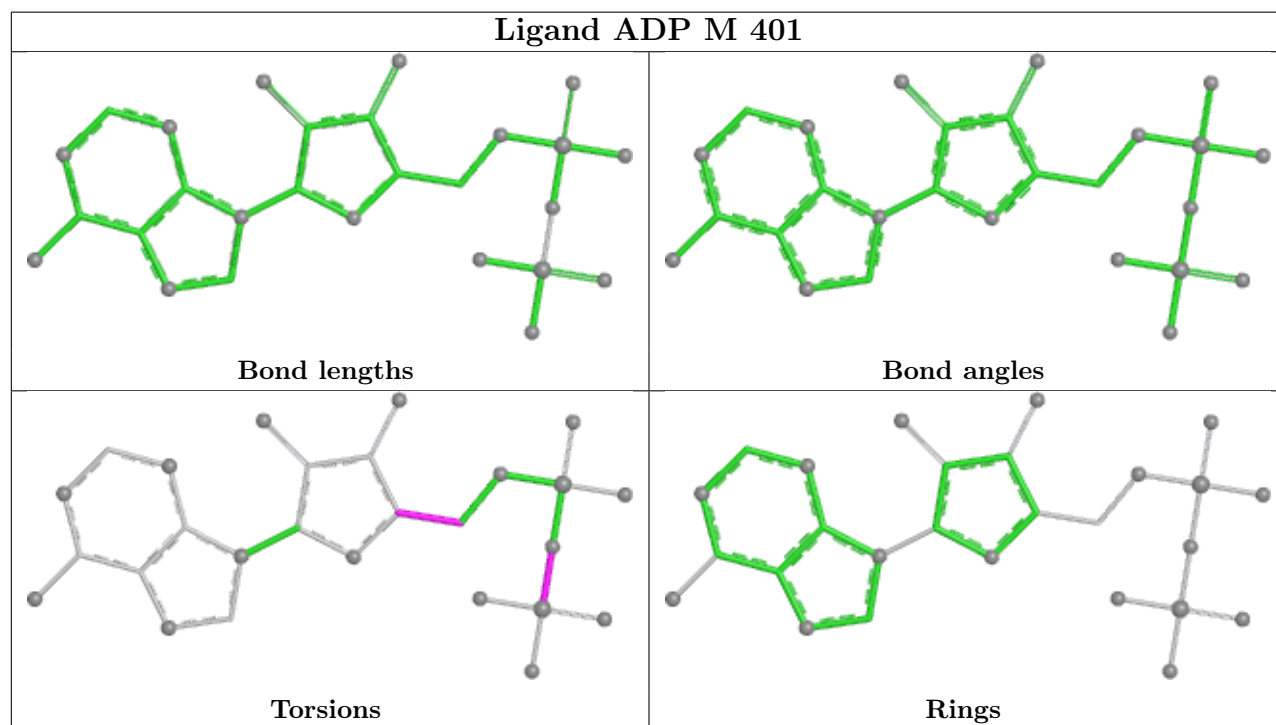
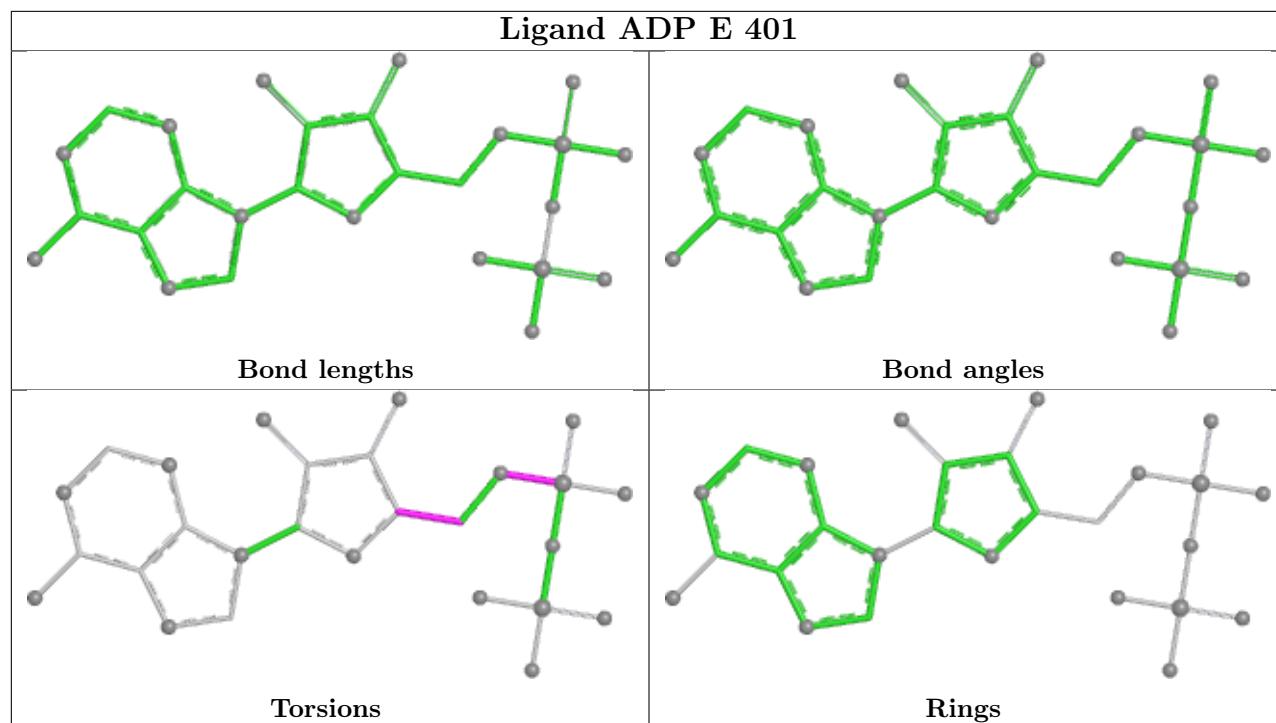
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

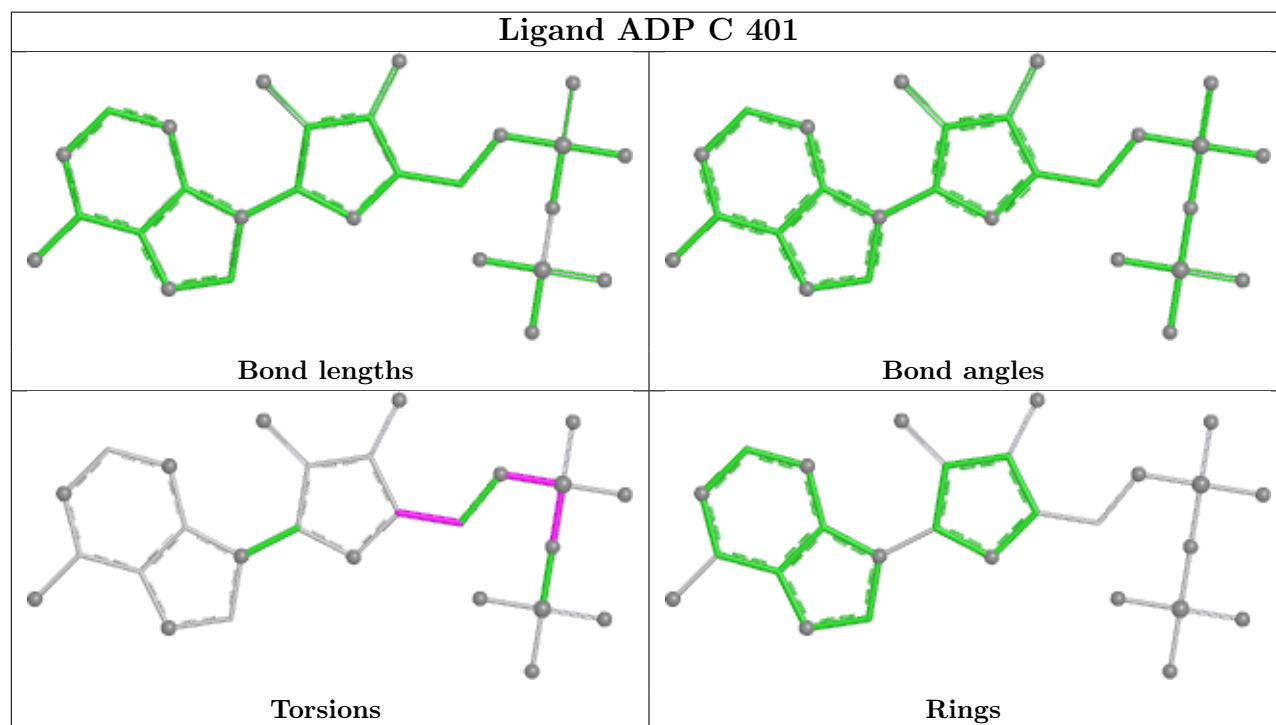
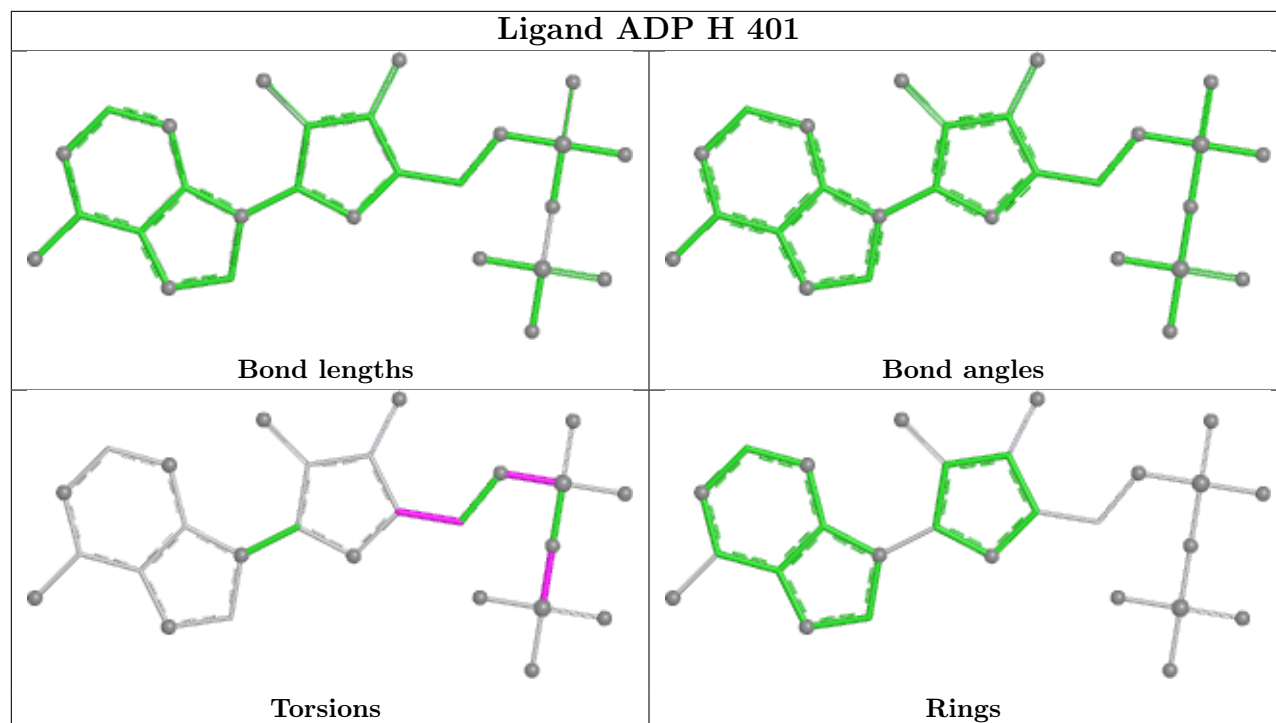
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

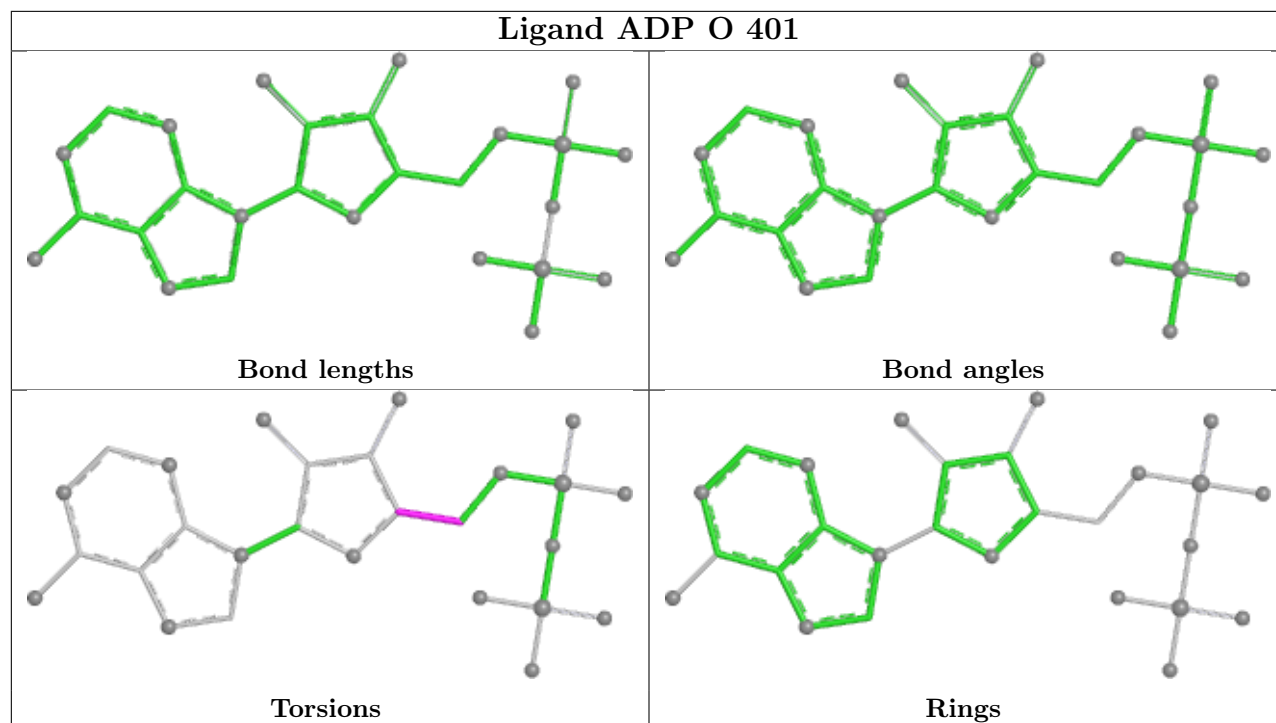












5.7 Other polymers [i](#)

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

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	290/309 (93%)	0.42	17 (5%)	28	22	36, 60, 117, 149	0
1	B	281/309 (90%)	0.42	21 (7%)	20	16	40, 58, 93, 134	0
1	C	282/309 (91%)	0.29	13 (4%)	37	29	38, 53, 96, 145	0
1	D	291/309 (94%)	0.32	11 (3%)	44	36	40, 54, 118, 156	0
1	E	292/309 (94%)	0.40	18 (6%)	26	21	32, 54, 113, 137	0
1	F	284/309 (91%)	0.37	17 (5%)	27	21	38, 58, 102, 170	0
1	G	282/309 (91%)	0.27	11 (3%)	43	35	33, 51, 93, 146	0
1	H	284/309 (91%)	0.34	15 (5%)	32	25	36, 53, 103, 159	0
1	I	282/309 (91%)	0.37	11 (3%)	43	35	42, 63, 108, 165	0
1	J	286/309 (92%)	0.40	14 (4%)	35	27	42, 61, 110, 182	0
1	K	283/309 (91%)	0.31	11 (3%)	43	35	37, 58, 108, 162	0
1	L	294/309 (95%)	0.50	18 (6%)	27	21	46, 66, 124, 165	0
1	M	290/309 (93%)	0.68	18 (6%)	26	21	45, 75, 131, 168	0
1	N	290/309 (93%)	1.13	36 (12%)	8	7	60, 95, 147, 199	0
1	O	290/309 (93%)	0.47	19 (6%)	24	19	46, 66, 122, 156	0
1	P	286/309 (92%)	0.48	21 (7%)	21	17	44, 64, 115, 158	0
All	All	4587/4944 (92%)	0.45	271 (5%)	28	22	32, 61, 119, 199	0

The worst 5 of 271 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	214	LEU	5.6
1	J	210	PHE	4.8
1	D	146	THR	4.7
1	G	69	VAL	4.5
1	B	147	GLN	4.5

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](#)

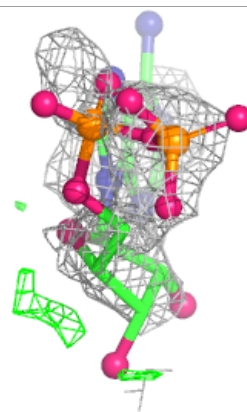
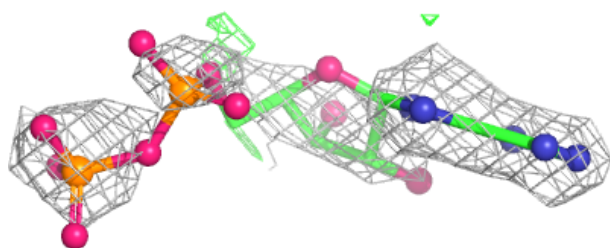
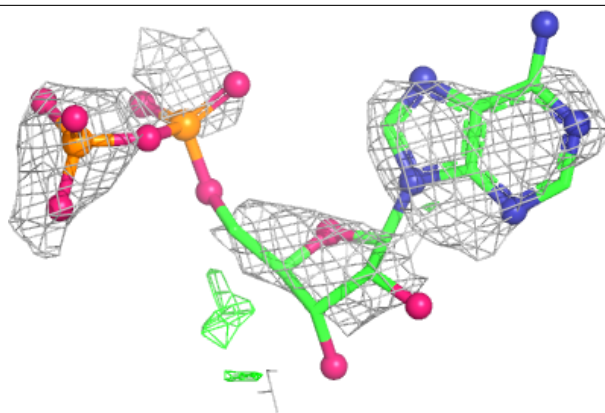
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ADP	B	401	27/27	0.73	0.21	87,105,118,121	27
2	ADP	K	401	27/27	0.75	0.21	84,101,123,126	27
2	ADP	J	401	27/27	0.79	0.15	66,75,92,93	27
2	ADP	A	401	27/27	0.79	0.18	71,81,85,87	27
2	ADP	C	401	27/27	0.80	0.18	66,78,97,97	27
2	ADP	M	401	27/27	0.80	0.16	69,83,92,94	27
2	ADP	G	401	27/27	0.83	0.16	62,74,91,92	27
2	ADP	O	401	27/27	0.83	0.16	72,88,111,113	27
2	ADP	H	401	27/27	0.84	0.16	72,82,94,96	27
2	ADP	E	401	27/27	0.87	0.15	64,78,85,86	27
2	ADP	D	401	27/27	0.88	0.13	72,84,104,105	27

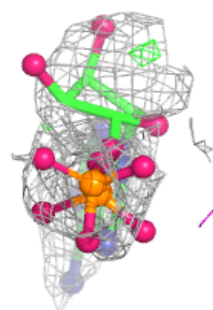
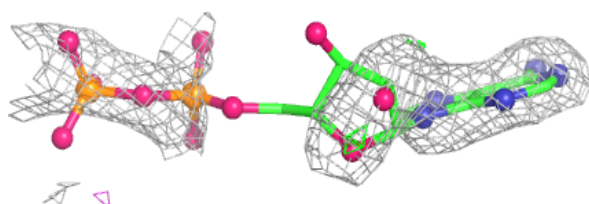
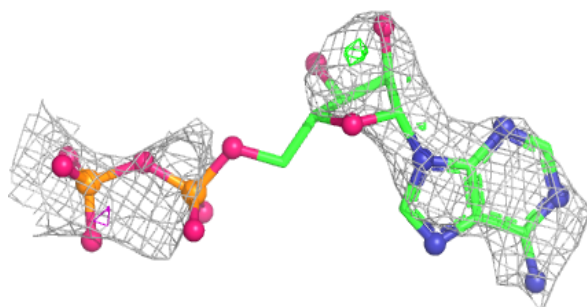
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP B 401:

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

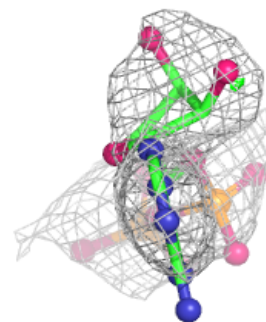
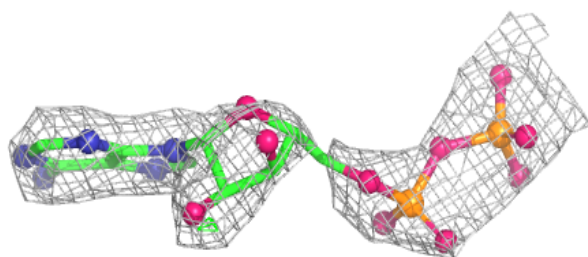
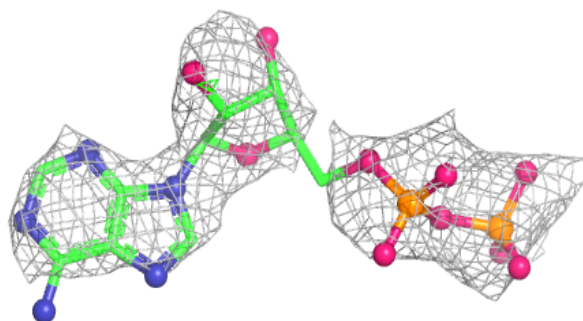
**Electron density around ADP K 401:**

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

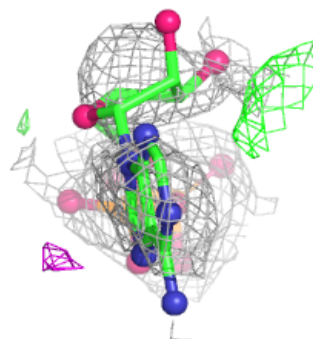
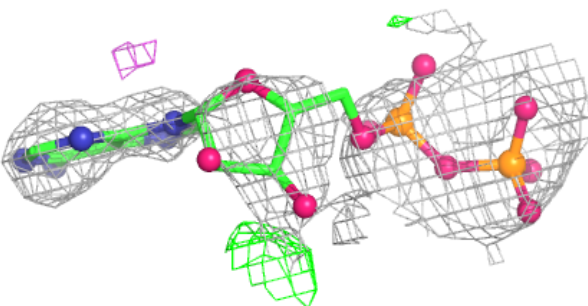
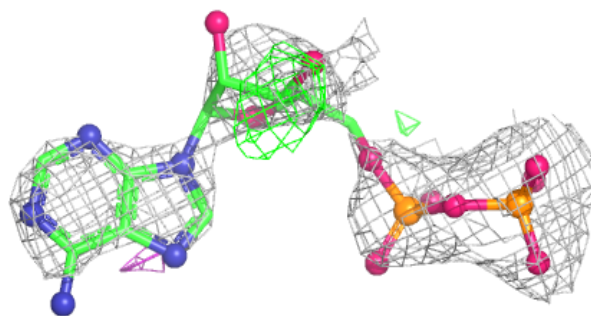


Electron density around ADP J 401:

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

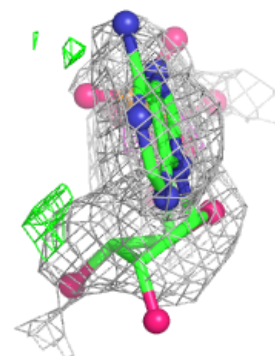
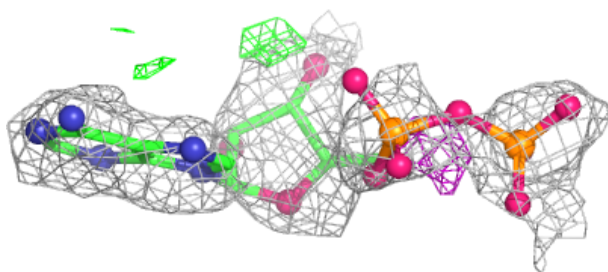
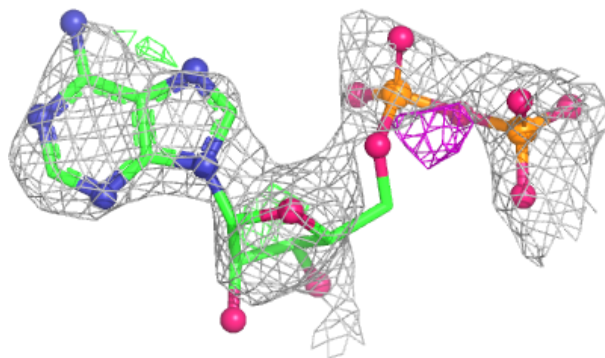
**Electron density around ADP A 401:**

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

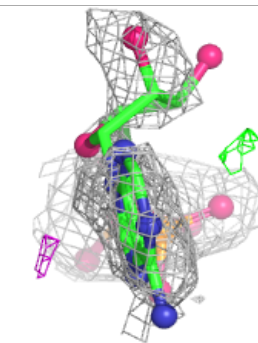
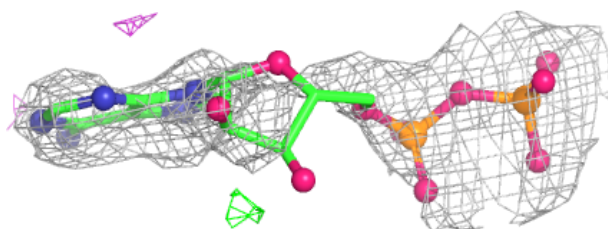
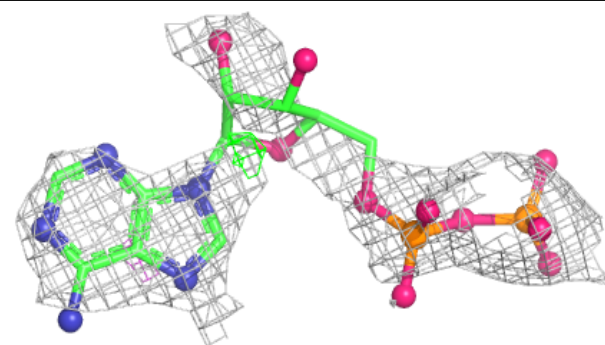


Electron density around ADP C 401:

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

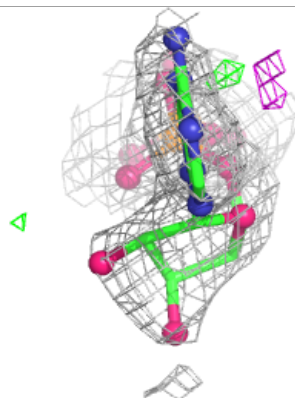
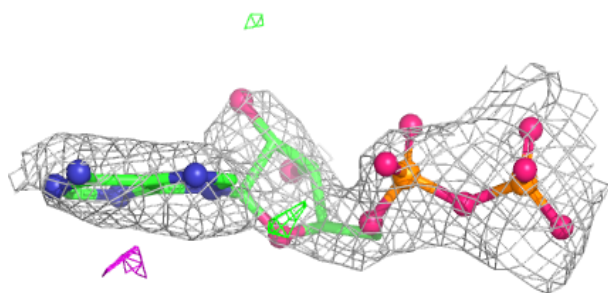
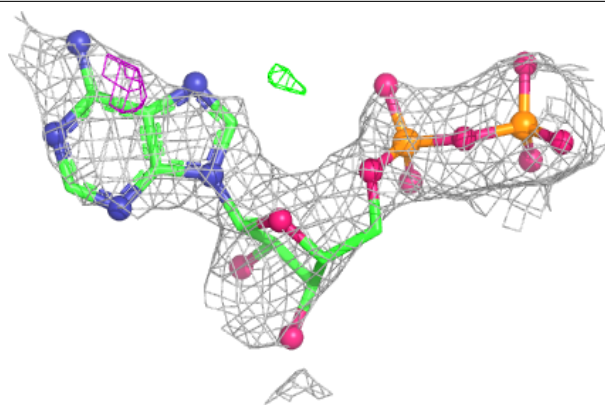
**Electron density around ADP M 401:**

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

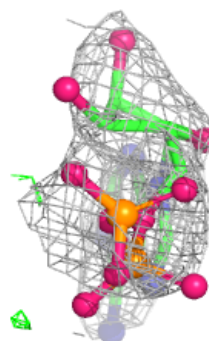
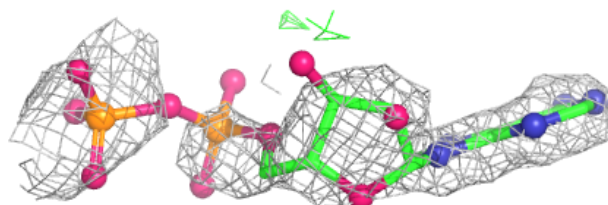
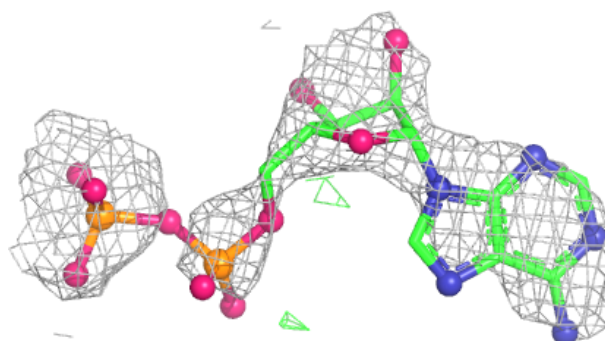


Electron density around ADP G 401:

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

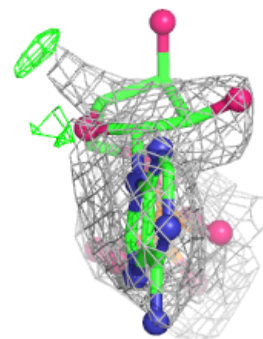
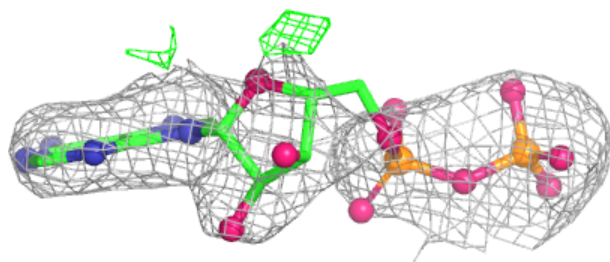
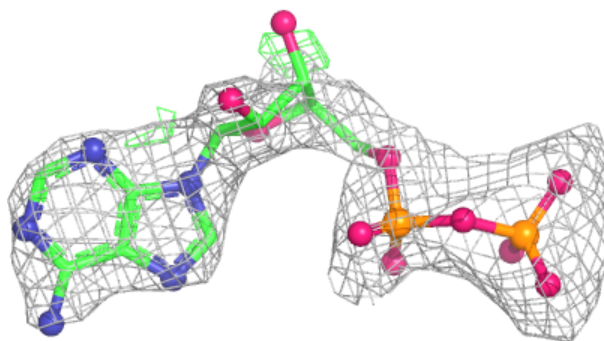
**Electron density around ADP O 401:**

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

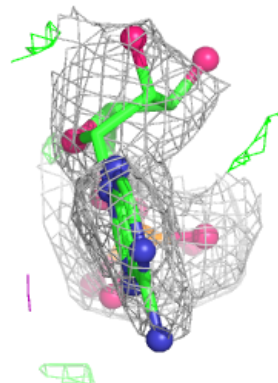
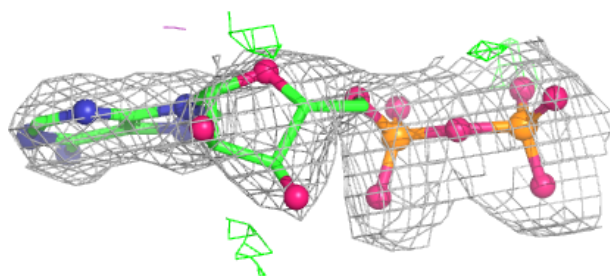
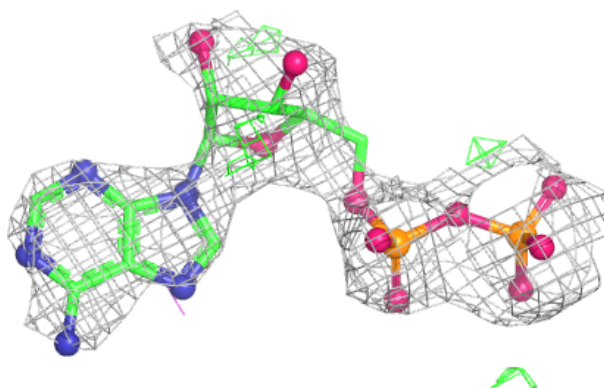


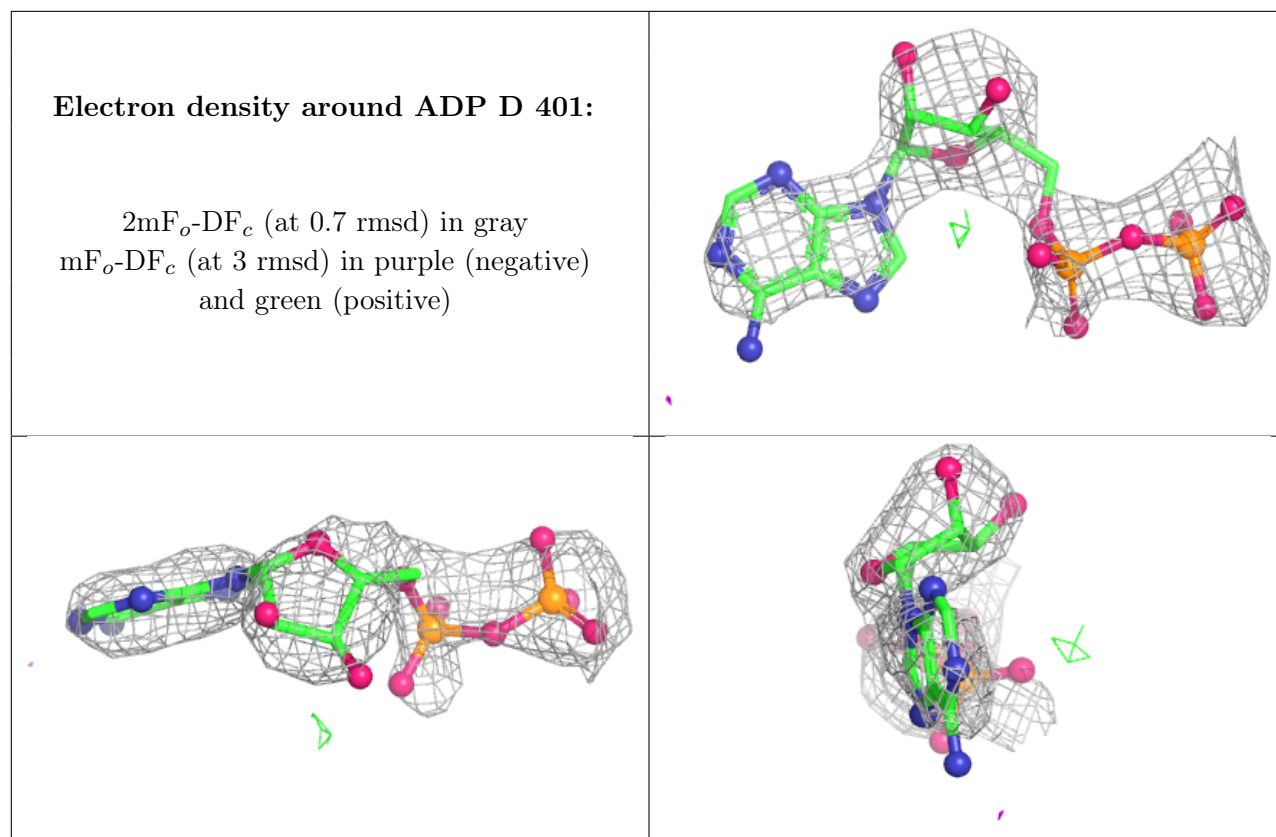
Electron density around ADP H 401:

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

**Electron density around ADP E 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.