



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:54 AM UTC

PDB ID : 3UK6 / pdb_00003uk6
Title : Crystal Structure of the Tip48 (Tip49b) hexamer
Authors : Petukhov, M.; Dagkessamanskaja, A.; Bommer, M.; Barrett, T.; Tsaneva, I.; Yakimov, A.; Queval, R.; Shvetsov, A.; Khodorkovskiy, M.; Kas, E.; Grigoriev, M.
Deposited on : 2011-11-09
Resolution : 2.95 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

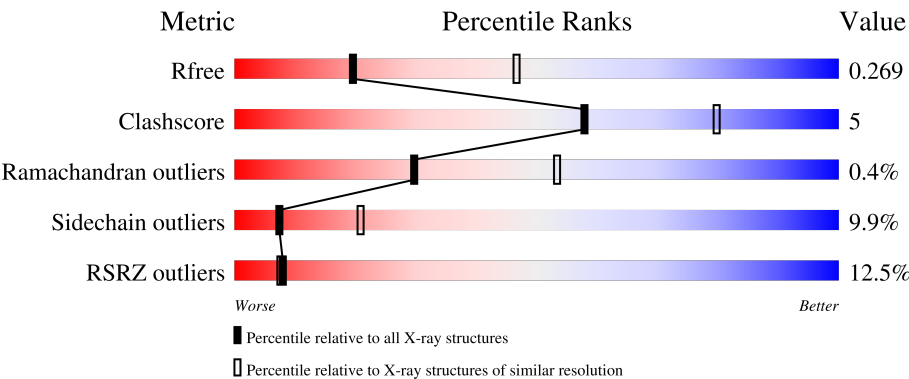
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	368	6% 71% 9% • 19%
1	B	368	7% 71% 8% • 18%
1	C	368	4% 75% 11% • 13%
1	D	368	7% 71% 9% • 19%

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Mol	Chain	Length	Quality of chain
1	E	368	
1	F	368	
1	G	368	
1	H	368	
1	I	368	
1	J	368	
1	K	368	
1	L	368	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 22870 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 RuvB-like 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	0	0	0
			1944	1211	345	379	9			
1	B	300	Total	C	N	O	S	0	0	0
			1962	1228	350	377	7			
1	C	321	Total	C	N	O	S	0	0	0
			2117	1324	372	412	9			
1	D	299	Total	C	N	O	S	0	0	0
			1932	1211	341	371	9			
1	E	290	Total	C	N	O	S	0	0	0
			1886	1178	331	368	9			
1	F	301	Total	C	N	O	S	0	0	0
			1964	1232	346	377	9			
1	G	330	Total	C	N	O	S	0	0	0
			2182	1368	387	417	10			
1	H	277	Total	C	N	O	S	0	0	0
			1731	1083	304	339	5			
1	I	294	Total	C	N	O	S	0	0	0
			1829	1140	323	359	7			
1	J	300	Total	C	N	O	S	0	0	0
			1857	1155	337	360	5			
1	K	283	Total	C	N	O	S	0	0	0
			1752	1089	310	351	2			
1	L	233	Total	C	N	O	S	0	0	0
			1392	868	246	274	4			

There are 131 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	236	ALA	-	expression tag	UNP Q9Y230
A	237	GLY	-	expression tag	UNP Q9Y230
A	238	ALA	-	expression tag	UNP Q9Y230
A	464	LEU	-	expression tag	UNP Q9Y230
A	465	GLU	-	expression tag	UNP Q9Y230

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Chain	Residue	Modelled	Actual	Comment	Reference
A	466	HIS	-	expression tag	UNP Q9Y230
A	467	HIS	-	expression tag	UNP Q9Y230
A	468	HIS	-	expression tag	UNP Q9Y230
A	469	HIS	-	expression tag	UNP Q9Y230
A	470	HIS	-	expression tag	UNP Q9Y230
A	471	HIS	-	expression tag	UNP Q9Y230
B	236	ALA	-	expression tag	UNP Q9Y230
B	237	GLY	-	expression tag	UNP Q9Y230
B	238	ALA	-	expression tag	UNP Q9Y230
B	464	LEU	-	expression tag	UNP Q9Y230
B	465	GLU	-	expression tag	UNP Q9Y230
B	466	HIS	-	expression tag	UNP Q9Y230
B	467	HIS	-	expression tag	UNP Q9Y230
B	468	HIS	-	expression tag	UNP Q9Y230
B	469	HIS	-	expression tag	UNP Q9Y230
B	470	HIS	-	expression tag	UNP Q9Y230
B	471	HIS	-	expression tag	UNP Q9Y230
C	236	ALA	-	expression tag	UNP Q9Y230
C	237	GLY	-	expression tag	UNP Q9Y230
C	238	ALA	-	expression tag	UNP Q9Y230
C	465	GLU	-	expression tag	UNP Q9Y230
C	466	HIS	-	expression tag	UNP Q9Y230
C	467	HIS	-	expression tag	UNP Q9Y230
C	468	HIS	-	expression tag	UNP Q9Y230
C	469	HIS	-	expression tag	UNP Q9Y230
C	470	HIS	-	expression tag	UNP Q9Y230
C	471	HIS	-	expression tag	UNP Q9Y230
D	236	ALA	-	expression tag	UNP Q9Y230
D	237	GLY	-	expression tag	UNP Q9Y230
D	238	ALA	-	expression tag	UNP Q9Y230
D	464	LEU	-	expression tag	UNP Q9Y230
D	465	GLU	-	expression tag	UNP Q9Y230
D	466	HIS	-	expression tag	UNP Q9Y230
D	467	HIS	-	expression tag	UNP Q9Y230
D	468	HIS	-	expression tag	UNP Q9Y230
D	469	HIS	-	expression tag	UNP Q9Y230
D	470	HIS	-	expression tag	UNP Q9Y230
D	471	HIS	-	expression tag	UNP Q9Y230
E	236	ALA	-	expression tag	UNP Q9Y230
E	237	GLY	-	expression tag	UNP Q9Y230
E	238	ALA	-	expression tag	UNP Q9Y230
E	464	LEU	-	expression tag	UNP Q9Y230

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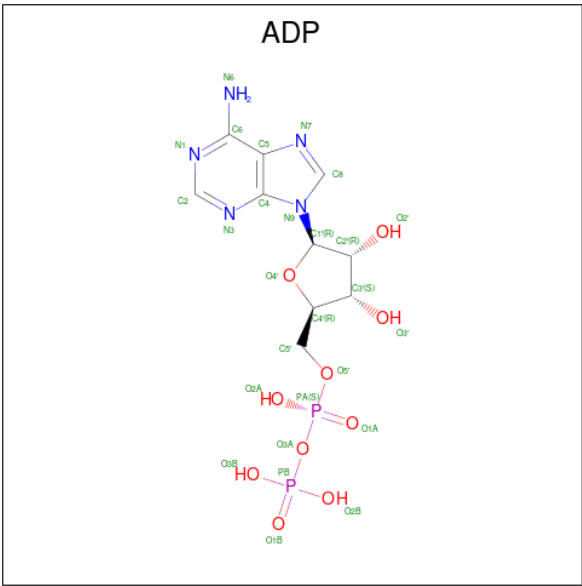
Chain	Residue	Modelled	Actual	Comment	Reference
E	465	GLU	-	expression tag	UNP Q9Y230
E	466	HIS	-	expression tag	UNP Q9Y230
E	467	HIS	-	expression tag	UNP Q9Y230
E	468	HIS	-	expression tag	UNP Q9Y230
E	469	HIS	-	expression tag	UNP Q9Y230
E	470	HIS	-	expression tag	UNP Q9Y230
E	471	HIS	-	expression tag	UNP Q9Y230
F	236	ALA	-	expression tag	UNP Q9Y230
F	237	GLY	-	expression tag	UNP Q9Y230
F	238	ALA	-	expression tag	UNP Q9Y230
F	464	LEU	-	expression tag	UNP Q9Y230
F	465	GLU	-	expression tag	UNP Q9Y230
F	466	HIS	-	expression tag	UNP Q9Y230
F	467	HIS	-	expression tag	UNP Q9Y230
F	468	HIS	-	expression tag	UNP Q9Y230
F	469	HIS	-	expression tag	UNP Q9Y230
F	470	HIS	-	expression tag	UNP Q9Y230
F	471	HIS	-	expression tag	UNP Q9Y230
G	236	ALA	-	expression tag	UNP Q9Y230
G	237	GLY	-	expression tag	UNP Q9Y230
G	238	ALA	-	expression tag	UNP Q9Y230
G	464	LEU	-	expression tag	UNP Q9Y230
G	465	GLU	-	expression tag	UNP Q9Y230
G	466	HIS	-	expression tag	UNP Q9Y230
G	467	HIS	-	expression tag	UNP Q9Y230
G	468	HIS	-	expression tag	UNP Q9Y230
G	469	HIS	-	expression tag	UNP Q9Y230
G	470	HIS	-	expression tag	UNP Q9Y230
G	471	HIS	-	expression tag	UNP Q9Y230
H	236	ALA	-	expression tag	UNP Q9Y230
H	237	GLY	-	expression tag	UNP Q9Y230
H	238	ALA	-	expression tag	UNP Q9Y230
H	464	LEU	-	expression tag	UNP Q9Y230
H	465	GLU	-	expression tag	UNP Q9Y230
H	466	HIS	-	expression tag	UNP Q9Y230
H	467	HIS	-	expression tag	UNP Q9Y230
H	468	HIS	-	expression tag	UNP Q9Y230
H	469	HIS	-	expression tag	UNP Q9Y230
H	470	HIS	-	expression tag	UNP Q9Y230
H	471	HIS	-	expression tag	UNP Q9Y230
I	236	ALA	-	expression tag	UNP Q9Y230
I	237	GLY	-	expression tag	UNP Q9Y230

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Chain	Residue	Modelled	Actual	Comment	Reference
I	238	ALA	-	expression tag	UNP Q9Y230
I	464	LEU	-	expression tag	UNP Q9Y230
I	465	GLU	-	expression tag	UNP Q9Y230
I	466	HIS	-	expression tag	UNP Q9Y230
I	467	HIS	-	expression tag	UNP Q9Y230
I	468	HIS	-	expression tag	UNP Q9Y230
I	469	HIS	-	expression tag	UNP Q9Y230
I	470	HIS	-	expression tag	UNP Q9Y230
I	471	HIS	-	expression tag	UNP Q9Y230
J	236	ALA	-	expression tag	UNP Q9Y230
J	237	GLY	-	expression tag	UNP Q9Y230
J	238	ALA	-	expression tag	UNP Q9Y230
J	464	LEU	-	expression tag	UNP Q9Y230
J	465	GLU	-	expression tag	UNP Q9Y230
J	466	HIS	-	expression tag	UNP Q9Y230
J	467	HIS	-	expression tag	UNP Q9Y230
J	468	HIS	-	expression tag	UNP Q9Y230
J	469	HIS	-	expression tag	UNP Q9Y230
J	470	HIS	-	expression tag	UNP Q9Y230
J	471	HIS	-	expression tag	UNP Q9Y230
K	236	ALA	-	expression tag	UNP Q9Y230
K	237	GLY	-	expression tag	UNP Q9Y230
K	238	ALA	-	expression tag	UNP Q9Y230
K	464	LEU	-	expression tag	UNP Q9Y230
K	465	GLU	-	expression tag	UNP Q9Y230
K	466	HIS	-	expression tag	UNP Q9Y230
K	467	HIS	-	expression tag	UNP Q9Y230
K	468	HIS	-	expression tag	UNP Q9Y230
K	469	HIS	-	expression tag	UNP Q9Y230
K	470	HIS	-	expression tag	UNP Q9Y230
K	471	HIS	-	expression tag	UNP Q9Y230
L	236	ALA	-	expression tag	UNP Q9Y230
L	237	GLY	-	expression tag	UNP Q9Y230
L	238	ALA	-	expression tag	UNP Q9Y230
L	464	LEU	-	expression tag	UNP Q9Y230
L	465	GLU	-	expression tag	UNP Q9Y230
L	466	HIS	-	expression tag	UNP Q9Y230
L	467	HIS	-	expression tag	UNP Q9Y230
L	468	HIS	-	expression tag	UNP Q9Y230
L	469	HIS	-	expression tag	UNP Q9Y230
L	470	HIS	-	expression tag	UNP Q9Y230
L	471	HIS	-	expression tag	UNP Q9Y230

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

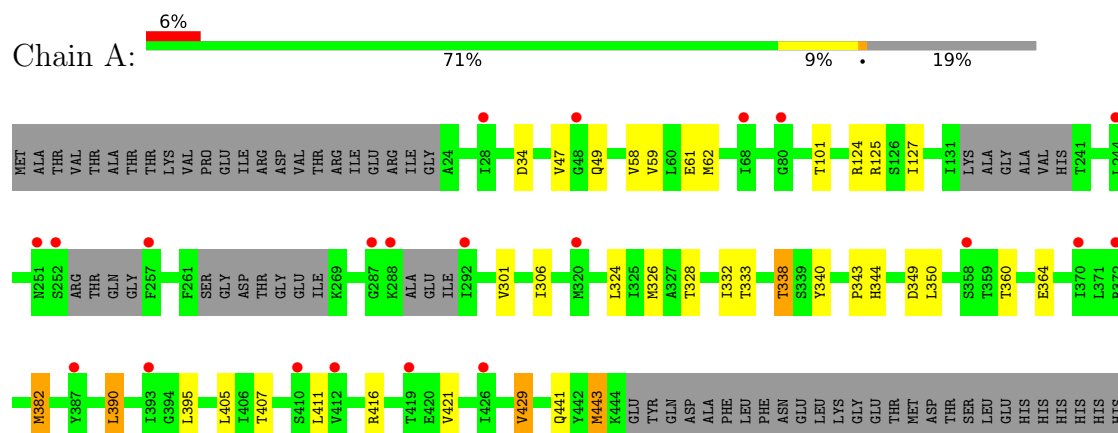


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	G	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	I	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
			25	9	5	9	2		
2	L	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

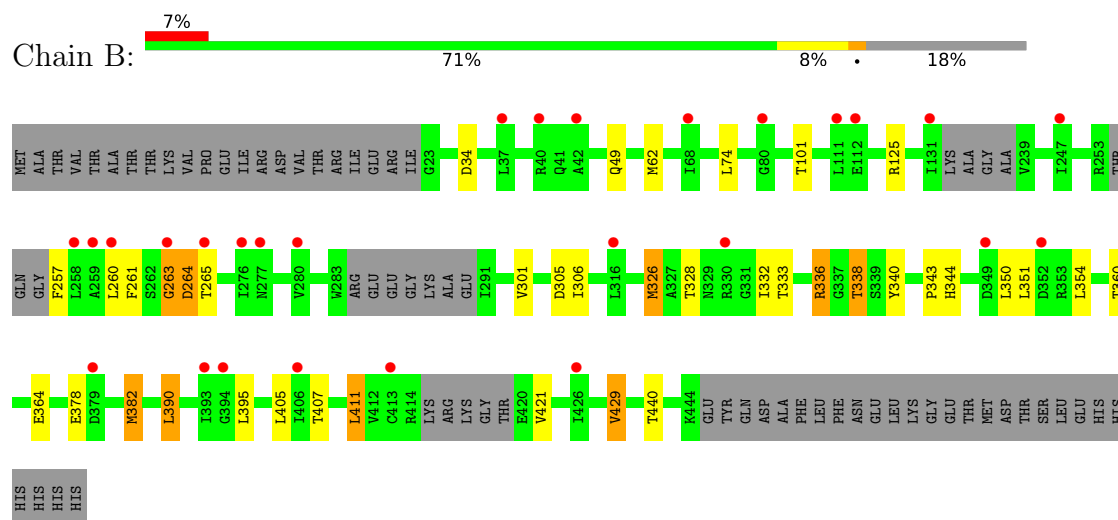
3 Residue-property plots [i](#)

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.

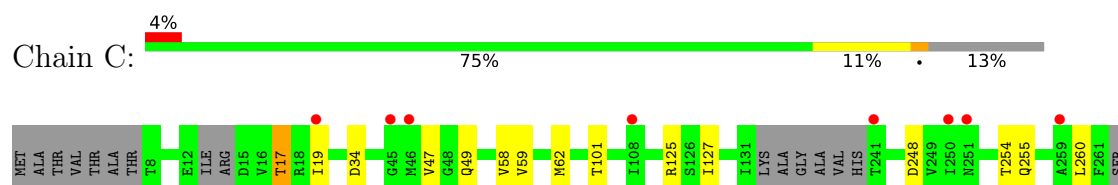
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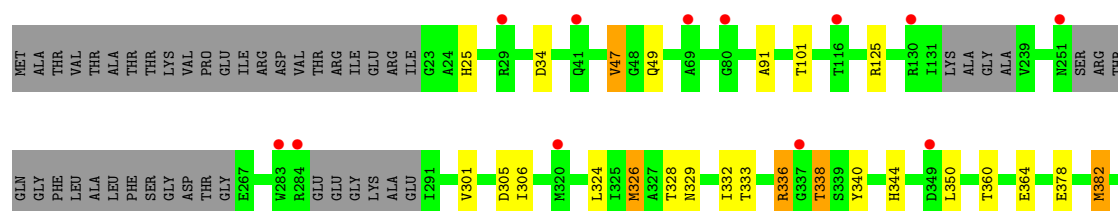


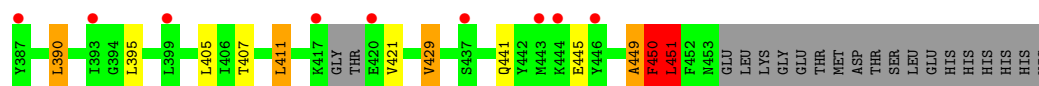
• Molecule 1: RuvB-like 2



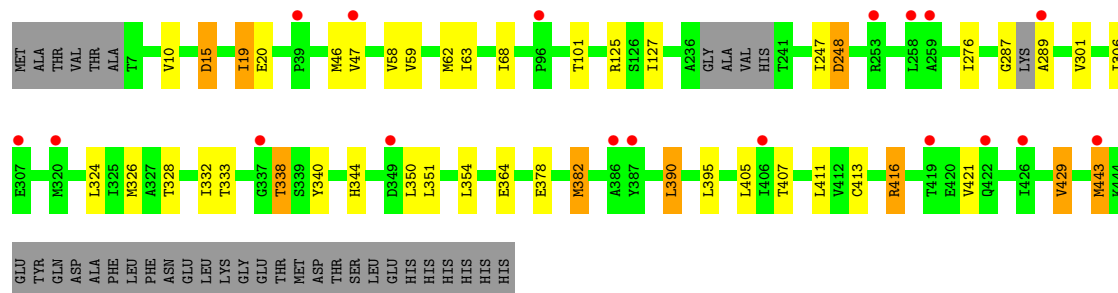
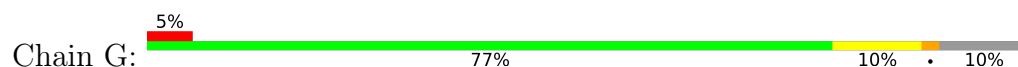
• Molecule 1: RuvB-like 2



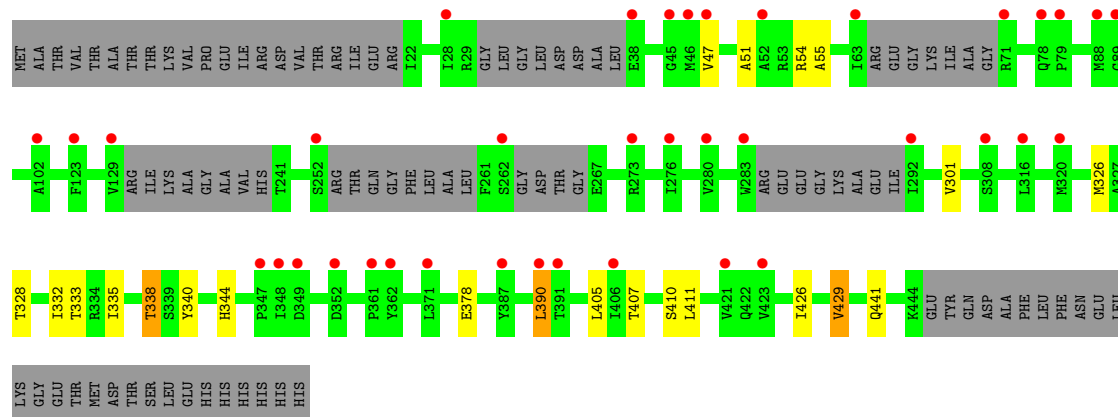




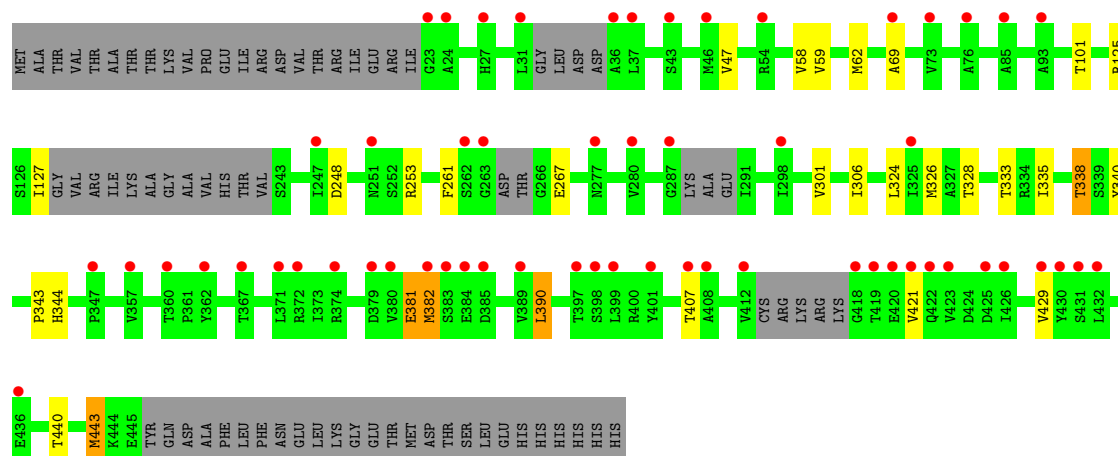
• Molecule 1: RuvB-like 2



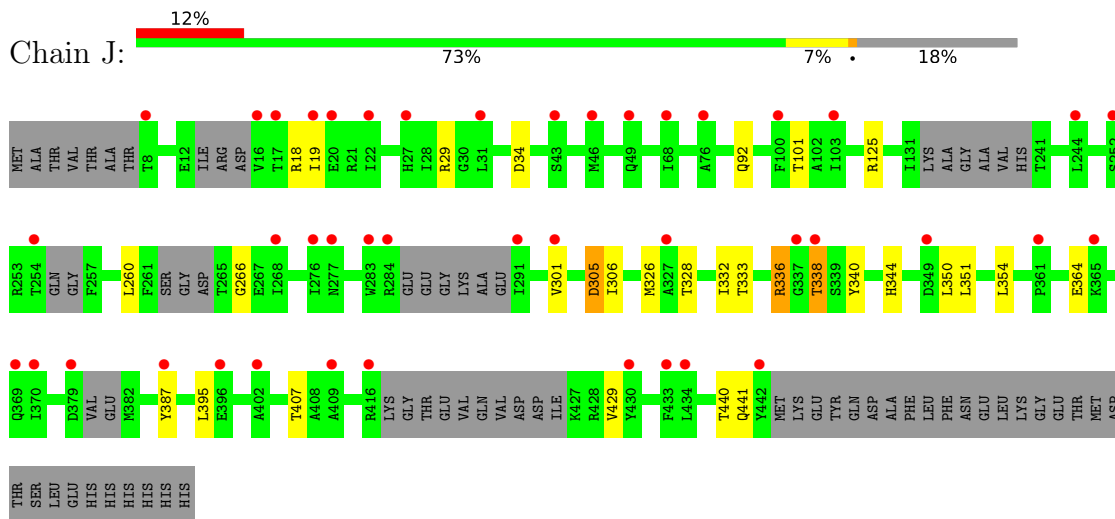
• Molecule 1: RuvB-like 2



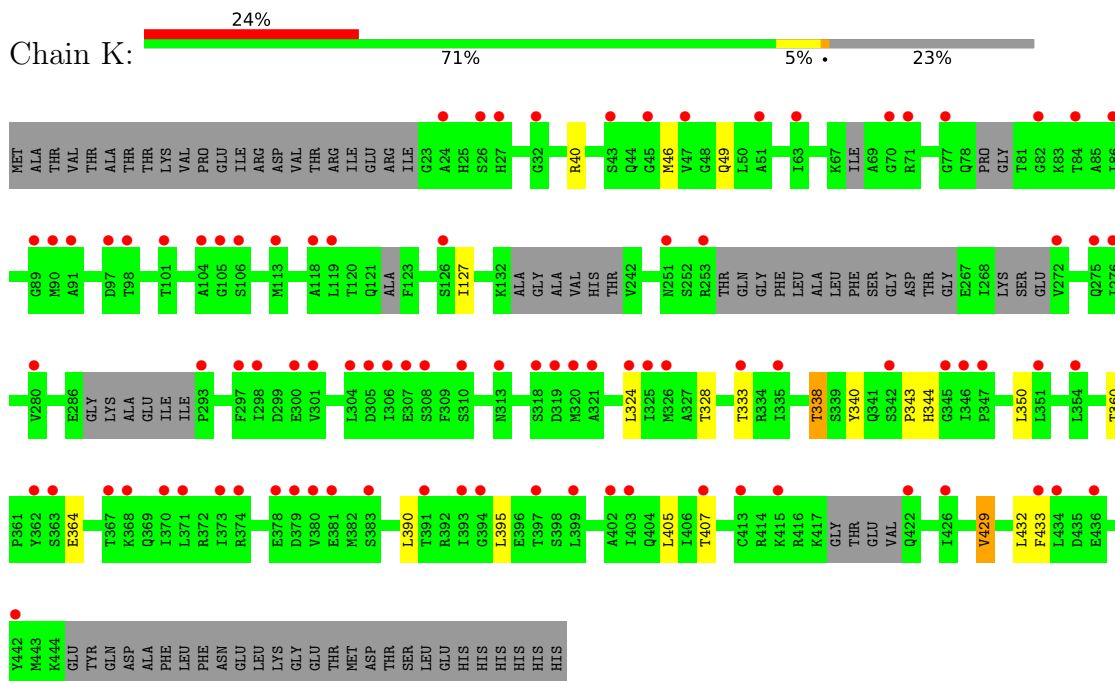
• Molecule 1: RuvB-like 2



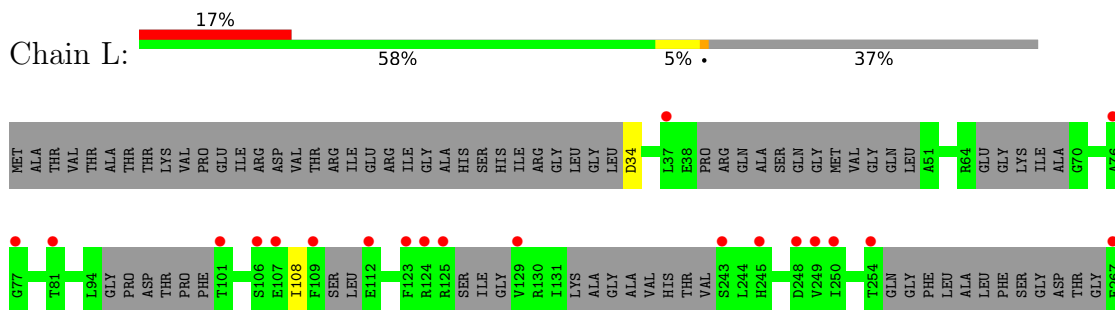
- Molecule 1: RuvB-like 2

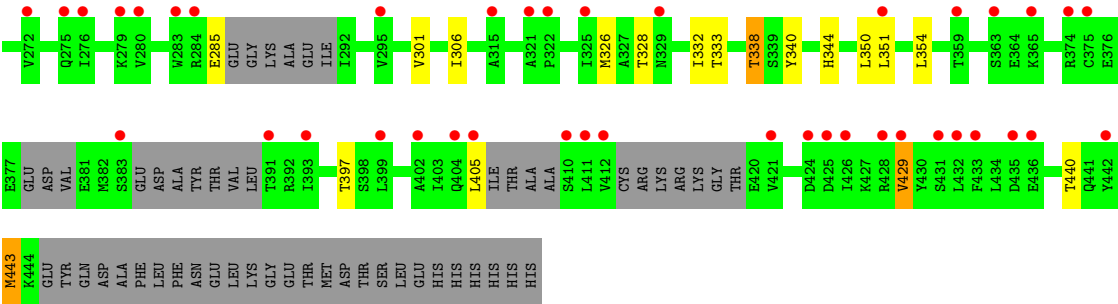


- Molecule 1: RuvB-like 2



- Molecule 1: RuvB-like 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	113.07Å 186.28Å 129.86Å 90.00° 108.95° 90.00°	Depositor
Resolution (Å)	43.19 – 2.95 43.19 – 2.95	Depositor EDS
% Data completeness (in resolution range)	97.1 (43.19-2.95) 97.0 (43.19-2.95)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.96Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.241 , 0.264 0.269 , 0.269	Depositor DCC
R_{free} test set	5179 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	80.1	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 140.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	22870	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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	0.91	0/1965	1.39	2/2683 (0.1%)
1	B	0.96	1/1985 (0.1%)	1.44	6/2713 (0.2%)
1	C	0.96	0/2145	1.43	6/2934 (0.2%)
1	D	0.91	0/1954	1.44	5/2671 (0.2%)
1	E	0.93	1/1907 (0.1%)	1.41	3/2607 (0.1%)
1	F	1.00	1/1986 (0.1%)	1.44	10/2716 (0.4%)
1	G	0.94	0/2210	1.42	4/3022 (0.1%)
1	H	0.88	0/1750	1.39	1/2402 (0.0%)
1	I	0.95	1/1850 (0.1%)	1.46	4/2534 (0.2%)
1	J	0.92	0/1876	1.41	4/2571 (0.2%)
1	K	0.92	0/1767	1.44	0/2426
1	L	0.91	1/1393 (0.1%)	1.41	3/1907 (0.2%)
All	All	0.93	5/22788 (0.0%)	1.43	48/31186 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	69	ALA	CA-C	7.09	1.61	1.52
1	B	326	MET	SD-CE	-6.94	1.62	1.79
1	F	326	MET	SD-CE	-6.67	1.62	1.79
1	L	397	THR	CA-C	5.48	1.55	1.52
1	E	326	MET	SD-CE	-5.05	1.67	1.79

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	20	GLU	N-CA-C	-10.31	100.37	113.16
1	I	69	ALA	CA-C-N	8.86	137.65	121.70
1	I	69	ALA	C-N-CA	8.86	137.65	121.70
1	D	263	GLY	CA-C-N	8.18	136.43	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	263	GLY	C-N-CA	8.18	136.43	121.70
1	E	378	GLU	CB-CG-CD	7.52	125.39	112.60
1	D	130	ARG	N-CA-C	6.78	119.48	108.63
1	B	265	THR	CA-C-N	6.64	133.66	121.70
1	B	265	THR	C-N-CA	6.64	133.66	121.70
1	C	17	THR	CB-CA-C	6.45	120.21	109.89
1	G	10	VAL	N-CA-C	6.13	114.22	108.15
1	F	450	PHE	N-CA-C	5.96	123.50	110.80
1	G	15	ASP	CA-CB-CG	5.86	118.46	112.60
1	C	19	ILE	N-CA-C	-5.67	106.29	112.80
1	C	248	ASP	CA-CB-CG	5.65	118.25	112.60
1	I	248	ASP	CA-CB-CG	5.63	118.23	112.60
1	G	248	ASP	CA-CB-CG	5.54	118.14	112.60
1	C	19	ILE	CA-C-N	5.49	128.65	120.31
1	C	19	ILE	C-N-CA	5.49	128.65	120.31
1	D	130	ARG	CA-C-N	5.48	131.56	121.70
1	D	130	ARG	C-N-CA	5.48	131.56	121.70
1	I	381	GLU	N-CA-CB	5.38	120.20	110.83
1	E	34	ASP	CA-CB-CG	5.33	117.93	112.60
1	J	34	ASP	CA-CB-CG	5.33	117.93	112.60
1	F	34	ASP	CA-CB-CG	5.28	117.88	112.60
1	B	264	ASP	CA-CB-CG	5.28	117.88	112.60
1	J	19	ILE	CA-C-N	5.23	129.46	120.72
1	J	19	ILE	C-N-CA	5.23	129.46	120.72
1	L	108	ILE	CA-C-N	5.22	131.10	121.70
1	L	108	ILE	C-N-CA	5.22	131.10	121.70
1	L	34	ASP	CA-CB-CG	5.19	117.79	112.60
1	F	25	HIS	CA-C-N	5.18	127.53	120.54
1	F	25	HIS	C-N-CA	5.18	127.53	120.54
1	A	349	ASP	CA-CB-CG	5.17	117.77	112.60
1	B	34	ASP	CA-CB-CG	5.14	117.75	112.60
1	H	335	ILE	N-CA-C	-5.12	100.95	108.54
1	A	34	ASP	CA-CB-CG	5.12	117.72	112.60
1	B	257	PHE	CA-C-N	5.11	130.90	121.70
1	B	257	PHE	C-N-CA	5.11	130.90	121.70
1	F	450	PHE	CA-CB-CG	5.11	118.91	113.80
1	F	449	ALA	CA-C-N	5.09	131.26	121.54
1	F	449	ALA	C-N-CA	5.09	131.26	121.54
1	F	451	LEU	N-CA-C	-5.07	106.94	112.72
1	J	305	ASP	CA-CB-CG	5.05	117.65	112.60
1	F	91	ALA	CA-C-N	5.02	127.00	120.28
1	F	91	ALA	C-N-CA	5.02	127.00	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	34	ASP	CA-CB-CG	5.00	117.60	112.60
1	E	50	LEU	N-CA-C	5.00	116.42	110.97

There are no chirality outliers.

There are no planarity outliers.

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	1944	0	1658	18	0
1	B	1962	0	1688	22	0
1	C	2117	0	1803	22	0
1	D	1932	0	1649	19	0
1	E	1886	0	1610	18	0
1	F	1964	0	1695	21	0
1	G	2182	0	1901	24	0
1	H	1731	0	1380	11	0
1	I	1829	0	1451	16	0
1	J	1857	0	1451	13	0
1	K	1752	0	1353	12	0
1	L	1392	0	1052	10	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	C	27	0	12	0	0
2	D	27	0	12	0	0
2	E	27	0	12	0	0
2	F	27	0	12	1	0
2	G	27	0	12	0	0
2	H	27	0	12	0	0
2	I	27	0	12	0	0
2	J	27	0	12	0	0
2	K	25	0	9	0	0
2	L	27	0	12	0	0
All	All	22870	0	18832	189	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 5.

All (189) 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:101:THR:HG21	1:I:125:ARG:HB3	1.58	0.83
1:A:101:THR:HG21	1:A:125:ARG:HB3	1.61	0.81
1:J:101:THR:HG21	1:J:125:ARG:HB3	1.60	0.81
1:E:101:THR:HG21	1:E:125:ARG:HB3	1.61	0.80
1:G:101:THR:HG21	1:G:125:ARG:HB3	1.62	0.80
1:B:101:THR:HG21	1:B:125:ARG:HB3	1.63	0.80
1:F:101:THR:HG21	1:F:125:ARG:HB3	1.62	0.80
1:C:101:THR:HG21	1:C:125:ARG:HB3	1.63	0.80
1:D:101:THR:HG21	1:D:125:ARG:HB3	1.65	0.77
1:D:389:VAL:HG11	1:F:451:LEU:HD23	1.69	0.74
1:A:382:MET:HG3	1:A:421:VAL:HB	1.74	0.70
1:E:382:MET:HG3	1:E:421:VAL:HB	1.74	0.70
1:B:263:GLY:H	1:B:264:ASP:HB3	1.57	0.69
1:C:382:MET:HG3	1:C:421:VAL:HB	1.76	0.68
1:F:382:MET:HG3	1:F:421:VAL:HB	1.75	0.67
1:B:382:MET:HG3	1:B:421:VAL:HB	1.76	0.67
1:I:382:MET:HG3	1:I:421:VAL:HB	1.77	0.66
1:H:328:THR:HG21	1:H:344:HIS:HB3	1.77	0.66
1:A:328:THR:HG21	1:A:344:HIS:HB3	1.78	0.65
1:J:328:THR:HG21	1:J:344:HIS:HB3	1.78	0.65
1:G:58:VAL:HG12	1:G:62:MET:HE2	1.78	0.65
1:D:328:THR:HG21	1:D:344:HIS:HB3	1.77	0.65
1:G:382:MET:HG3	1:G:421:VAL:HB	1.78	0.64
1:L:328:THR:HG21	1:L:344:HIS:HB3	1.79	0.64
1:D:382:MET:HG3	1:D:421:VAL:HB	1.78	0.64
1:G:248:ASP:HA	1:G:276:ILE:HD13	1.80	0.63
1:K:328:THR:HG21	1:K:344:HIS:HB3	1.78	0.63
1:F:301:VAL:HG21	1:F:326:MET:HE2	1.79	0.63
1:B:301:VAL:HG21	1:B:326:MET:HE2	1.80	0.63
1:E:301:VAL:HG21	1:E:326:MET:HE2	1.81	0.63
1:G:328:THR:HG21	1:G:344:HIS:HB3	1.80	0.62
1:B:328:THR:HG21	1:B:344:HIS:HB3	1.80	0.62
1:F:328:THR:HG21	1:F:344:HIS:HB3	1.81	0.62
1:E:328:THR:HG21	1:E:344:HIS:HB3	1.80	0.62
1:C:443:MET:HE3	1:C:443:MET:HA	1.82	0.62
1:C:301:VAL:HG21	1:C:326:MET:HE2	1.82	0.62
1:F:338:THR:CG2	1:F:340:TYR:H	2.14	0.61
1:C:328:THR:HG21	1:C:344:HIS:HB3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:THR:CG2	1:A:340:TYR:H	2.14	0.61
1:I:338:THR:CG2	1:I:340:TYR:H	2.14	0.60
1:C:58:VAL:HG12	1:C:62:MET:HE2	1.83	0.60
1:J:338:THR:CG2	1:J:340:TYR:H	2.15	0.60
1:I:301:VAL:HG21	1:I:326:MET:HE2	1.82	0.60
1:L:338:THR:CG2	1:L:340:TYR:H	2.15	0.60
1:C:338:THR:CG2	1:C:340:TYR:H	2.15	0.60
1:D:338:THR:CG2	1:D:340:TYR:H	2.14	0.60
1:K:405:LEU:HD22	1:K:429:VAL:HG13	1.84	0.60
1:B:338:THR:CG2	1:B:340:TYR:H	2.16	0.59
1:E:58:VAL:HG12	1:E:62:MET:HE2	1.85	0.59
1:I:58:VAL:HG12	1:I:62:MET:HE2	1.83	0.59
1:D:389:VAL:CG1	1:F:451:LEU:HD23	2.33	0.59
1:E:338:THR:CG2	1:E:340:TYR:H	2.14	0.59
1:H:301:VAL:HG21	1:H:326:MET:HE2	1.85	0.58
1:I:328:THR:HG21	1:I:344:HIS:HB3	1.83	0.58
1:K:343:PRO:HB3	1:L:440:THR:CG2	2.33	0.58
1:E:382:MET:HE1	1:E:390:LEU:HD12	1.86	0.58
1:D:382:MET:HE1	1:D:390:LEU:HD12	1.85	0.58
1:A:443:MET:HA	1:A:443:MET:HE3	1.85	0.58
1:J:301:VAL:HG21	1:J:326:MET:HE2	1.85	0.58
1:A:405:LEU:HD22	1:A:429:VAL:HG13	1.86	0.58
1:G:338:THR:CG2	1:G:340:TYR:H	2.17	0.58
1:G:301:VAL:HG21	1:G:326:MET:HE2	1.85	0.57
1:K:338:THR:CG2	1:K:340:TYR:H	2.16	0.57
1:L:301:VAL:HG21	1:L:326:MET:HE2	1.86	0.57
1:C:382:MET:HE1	1:C:390:LEU:HD12	1.87	0.57
1:H:338:THR:CG2	1:H:340:TYR:H	2.17	0.56
1:B:62:MET:HG3	1:C:411:LEU:HD13	1.87	0.56
1:A:343:PRO:HB3	1:B:440:THR:CG2	2.37	0.55
1:I:382:MET:HE1	1:I:390:LEU:HD12	1.89	0.55
1:B:405:LEU:HD22	1:B:429:VAL:HG13	1.89	0.55
1:D:301:VAL:HG21	1:D:326:MET:HE2	1.89	0.55
1:E:61:GLU:CB	1:F:411:LEU:HD21	2.36	0.54
1:I:381:GLU:CD	1:I:382:MET:H	2.16	0.54
1:I:338:THR:HG22	1:I:340:TYR:H	1.72	0.54
1:E:405:LEU:HD22	1:E:429:VAL:HG13	1.90	0.54
1:G:247:ILE:HG22	1:G:276:ILE:HG12	1.88	0.54
1:K:49:GLN:HE22	1:K:360:THR:H	1.55	0.54
1:D:338:THR:HG22	1:D:340:TYR:H	1.73	0.54
1:D:263:GLY:HA3	1:D:264:ASP:CB	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:368:LYS:CB	1:C:391:THR:HG21	2.39	0.52
1:A:301:VAL:HG21	1:A:326:MET:HE2	1.92	0.52
1:A:382:MET:HE1	1:A:390:LEU:HD12	1.91	0.52
1:F:405:LEU:HD22	1:F:429:VAL:HG13	1.91	0.52
1:L:338:THR:HG22	1:L:340:TYR:H	1.75	0.52
1:A:58:VAL:HG12	1:A:62:MET:HE2	1.91	0.52
1:C:49:GLN:HE22	1:C:360:THR:H	1.57	0.52
1:D:405:LEU:HD22	1:D:429:VAL:HG13	1.91	0.52
1:C:405:LEU:HD22	1:C:429:VAL:HG13	1.92	0.52
1:A:338:THR:HG22	1:A:340:TYR:H	1.75	0.51
1:F:338:THR:HG22	1:F:340:TYR:H	1.75	0.51
1:A:49:GLN:HE22	1:A:360:THR:H	1.56	0.51
1:J:338:THR:HG22	1:J:340:TYR:H	1.76	0.51
1:F:382:MET:HE1	1:F:390:LEU:HD12	1.91	0.51
1:L:405:LEU:HD22	1:L:429:VAL:HG13	1.92	0.51
1:L:443:MET:HE3	1:L:443:MET:HA	1.92	0.51
1:B:338:THR:HG22	1:B:340:TYR:H	1.75	0.51
1:A:61:GLU:CB	1:B:411:LEU:HD21	2.41	0.51
1:B:382:MET:HE1	1:B:390:LEU:HD12	1.93	0.51
1:H:405:LEU:HD22	1:H:429:VAL:HG13	1.92	0.50
1:C:368:LYS:HA	1:C:391:THR:CG2	2.41	0.50
1:J:29:ARG:HA	1:J:92:GLN:HE21	1.76	0.50
1:K:338:THR:HG22	1:K:340:TYR:H	1.75	0.50
1:E:338:THR:HG23	1:E:340:TYR:H	1.75	0.50
1:E:49:GLN:HE22	1:E:360:THR:H	1.59	0.50
1:G:19:ILE:H	1:G:19:ILE:HD12	1.77	0.50
1:A:124:ARG:HD2	1:B:261:PHE:O	2.13	0.49
1:F:301:VAL:HG21	1:F:326:MET:CE	2.42	0.49
1:H:54:ARG:HH11	1:K:432:LEU:HD21	1.77	0.49
1:F:49:GLN:HE22	1:F:360:THR:H	1.60	0.49
1:I:343:PRO:HB3	1:J:440:THR:CG2	2.43	0.49
1:F:329:ASN:HA	1:G:443:MET:HE2	1.93	0.49
1:F:450:PHE:CD1	1:F:450:PHE:C	2.90	0.49
1:G:405:LEU:HD22	1:G:429:VAL:HG13	1.95	0.49
1:H:338:THR:HG22	1:H:340:TYR:H	1.75	0.49
1:C:338:THR:HG23	1:C:340:TYR:H	1.77	0.49
1:D:364:GLU:HA	1:D:395:LEU:HD11	1.95	0.49
1:C:351:LEU:HD23	1:C:354:LEU:HD12	1.96	0.48
1:G:382:MET:HE1	1:G:390:LEU:HD12	1.96	0.48
1:G:338:THR:HG23	1:G:340:TYR:H	1.79	0.48
1:I:59:VAL:HA	1:I:62:MET:HE3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:VAL:HG21	1:B:326:MET:CE	2.43	0.47
1:G:443:MET:HE3	1:G:443:MET:HA	1.96	0.47
1:F:338:THR:HG23	1:F:340:TYR:H	1.79	0.47
1:I:443:MET:HA	1:I:443:MET:HE3	1.95	0.47
1:J:364:GLU:HA	1:J:395:LEU:HD11	1.97	0.47
1:C:338:THR:HG22	1:C:340:TYR:H	1.79	0.47
1:G:59:VAL:HA	1:G:62:MET:HE3	1.96	0.47
1:D:49:GLN:HE22	1:D:360:THR:H	1.62	0.47
1:J:338:THR:HG23	1:J:340:TYR:H	1.80	0.46
1:E:301:VAL:HG21	1:E:326:MET:CE	2.45	0.46
1:H:390:LEU:HG	1:H:426:ILE:HD12	1.96	0.46
1:C:382:MET:HE2	1:C:387:TYR:CD1	2.50	0.46
1:A:59:VAL:HA	1:A:62:MET:HE3	1.98	0.46
1:F:364:GLU:HA	1:F:395:LEU:HD11	1.98	0.46
1:L:338:THR:HG23	1:L:340:TYR:H	1.81	0.46
1:E:338:THR:HG22	1:E:340:TYR:H	1.79	0.46
1:D:343:PRO:HB3	1:I:440:THR:CG2	2.46	0.46
1:E:59:VAL:HA	1:E:62:MET:HE3	1.98	0.46
1:A:338:THR:HG23	1:A:340:TYR:H	1.80	0.45
1:G:338:THR:HG22	1:G:340:TYR:H	1.82	0.45
1:J:351:LEU:HD23	1:J:354:LEU:HD12	1.99	0.45
1:K:364:GLU:HA	1:K:395:LEU:HD11	1.98	0.45
1:B:49:GLN:HE22	1:B:360:THR:H	1.64	0.45
1:B:343:PRO:HB2	1:B:351:LEU:HD11	1.99	0.45
1:G:287:GLY:O	1:G:289:ALA:N	2.50	0.45
1:J:305:ASP:HA	1:J:336:ARG:HB2	1.98	0.45
1:L:351:LEU:HD23	1:L:354:LEU:HD12	1.99	0.45
1:F:450:PHE:C	1:F:450:PHE:HD1	2.25	0.45
1:E:364:GLU:HA	1:E:395:LEU:HD11	1.99	0.44
1:C:301:VAL:HG21	1:C:326:MET:CE	2.47	0.44
1:C:364:GLU:HA	1:C:395:LEU:HD11	1.99	0.44
1:E:305:ASP:HA	1:E:336:ARG:HB2	1.99	0.44
1:B:338:THR:HG23	1:B:340:TYR:H	1.83	0.44
1:D:351:LEU:HD23	1:D:354:LEU:HD12	2.00	0.43
1:G:301:VAL:HG21	1:G:326:MET:CE	2.48	0.43
1:B:305:ASP:HA	1:B:336:ARG:HB2	2.01	0.43
1:I:338:THR:HG23	1:I:340:TYR:H	1.83	0.43
1:D:305:ASP:HA	1:D:336:ARG:HB2	2.01	0.43
1:G:351:LEU:HD23	1:G:354:LEU:HD12	2.00	0.43
1:G:364:GLU:HA	1:G:395:LEU:HD11	2.00	0.43
1:I:335:ILE:O	1:I:338:THR:HB	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:GLU:HA	1:A:395:LEU:HD11	2.01	0.43
1:G:63:ILE:HG12	1:G:68:ILE:HG21	2.01	0.43
1:H:54:ARG:HD2	1:K:432:LEU:HD21	2.01	0.42
1:G:248:ASP:HA	1:G:276:ILE:CD1	2.46	0.42
1:F:305:ASP:HA	1:F:336:ARG:HB2	2.00	0.42
1:B:364:GLU:HA	1:B:395:LEU:HD11	2.01	0.42
1:E:382:MET:HE2	1:E:387:TYR:CD1	2.55	0.42
1:L:301:VAL:HG21	1:L:326:MET:CE	2.48	0.42
1:D:124:ARG:HD2	1:I:261:PHE:O	2.19	0.42
1:C:59:VAL:HA	1:C:62:MET:HE3	2.01	0.42
1:B:74:LEU:HB2	1:B:354:LEU:HD13	2.02	0.41
1:F:47:VAL:O	2:F:1450:ADP:N6	2.53	0.41
1:G:19:ILE:HD12	1:G:19:ILE:N	2.35	0.41
1:H:55:ALA:HB1	1:K:433:PHE:CE2	2.55	0.41
1:K:338:THR:HG23	1:K:340:TYR:H	1.84	0.41
1:J:387:TYR:HD1	1:J:387:TYR:HA	1.70	0.41
1:B:343:PRO:HB3	1:C:440:THR:CG2	2.50	0.41
1:F:390:LEU:HD23	1:F:390:LEU:HA	1.91	0.41
1:H:301:VAL:HG21	1:H:326:MET:CE	2.50	0.41
1:A:301:VAL:HG21	1:A:326:MET:CE	2.50	0.41
1:G:413:CYS:O	1:G:416:ARG:HG3	2.20	0.41
1:J:301:VAL:HG21	1:J:326:MET:CE	2.49	0.41
1:C:443:MET:HA	1:C:443:MET:CE	2.46	0.41
1:D:301:VAL:HG21	1:D:326:MET:CE	2.50	0.40
1:D:338:THR:HG23	1:D:340:TYR:H	1.81	0.40
1:E:351:LEU:HD23	1:E:354:LEU:HD12	2.02	0.40
1:H:51:ALA:O	1:K:432:LEU:HD22	2.22	0.40
1:B:390:LEU:HD23	1:B:390:LEU:HA	1.92	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	288/368 (78%)	283 (98%)	5 (2%)	0	100	100
1	B	290/368 (79%)	280 (97%)	9 (3%)	1 (0%)	36	59
1	C	313/368 (85%)	304 (97%)	7 (2%)	2 (1%)	21	45
1	D	289/368 (78%)	278 (96%)	8 (3%)	3 (1%)	12	32
1	E	280/368 (76%)	275 (98%)	5 (2%)	0	100	100
1	F	291/368 (79%)	280 (96%)	8 (3%)	3 (1%)	12	32
1	G	324/368 (88%)	312 (96%)	12 (4%)	0	100	100
1	H	263/368 (72%)	259 (98%)	4 (2%)	0	100	100
1	I	282/368 (77%)	272 (96%)	9 (3%)	1 (0%)	30	53
1	J	284/368 (77%)	276 (97%)	6 (2%)	2 (1%)	18	40
1	K	265/368 (72%)	261 (98%)	4 (2%)	0	100	100
1	L	207/368 (56%)	203 (98%)	4 (2%)	0	100	100
All	All	3376/4416 (76%)	3283 (97%)	81 (2%)	12 (0%)	30	53

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	255	GLN
1	D	264	ASP
1	F	450	PHE
1	D	254	THR
1	F	445	GLU
1	J	266	GLY
1	I	253	ARG
1	C	254	THR
1	D	255	GLN
1	F	449	ALA
1	J	18	ARG
1	B	263	GLY

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	153/307 (50%)	137 (90%)	16 (10%)	6	19
1	B	155/307 (50%)	142 (92%)	13 (8%)	10	26
1	C	168/307 (55%)	149 (89%)	19 (11%)	5	17
1	D	150/307 (49%)	135 (90%)	15 (10%)	7	20
1	E	149/307 (48%)	134 (90%)	15 (10%)	7	20
1	F	156/307 (51%)	139 (89%)	17 (11%)	6	18
1	G	175/307 (57%)	156 (89%)	19 (11%)	6	18
1	H	122/307 (40%)	111 (91%)	11 (9%)	9	24
1	I	125/307 (41%)	113 (90%)	12 (10%)	8	22
1	J	122/307 (40%)	112 (92%)	10 (8%)	10	27
1	K	116/307 (38%)	106 (91%)	10 (9%)	10	25
1	L	84/307 (27%)	76 (90%)	8 (10%)	8	22
All	All	1675/3684 (46%)	1510 (90%)	165 (10%)	7	21

All (165) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	VAL
1	A	127	ILE
1	A	306	ILE
1	A	324	LEU
1	A	332	ILE
1	A	333	THR
1	A	338	THR
1	A	350	LEU
1	A	382	MET
1	A	390	LEU
1	A	407	THR
1	A	411	LEU
1	A	416	ARG
1	A	429	VAL
1	A	441	GLN
1	A	443	MET
1	B	260	LEU
1	B	306	ILE
1	B	332	ILE
1	B	333	THR
1	B	336	ARG
1	B	338	THR

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Mol	Chain	Res	Type
1	B	350	LEU
1	B	378	GLU
1	B	382	MET
1	B	390	LEU
1	B	407	THR
1	B	411	LEU
1	B	429	VAL
1	C	17	THR
1	C	47	VAL
1	C	127	ILE
1	C	260	LEU
1	C	306	ILE
1	C	324	LEU
1	C	332	ILE
1	C	333	THR
1	C	338	THR
1	C	350	LEU
1	C	378	GLU
1	C	382	MET
1	C	390	LEU
1	C	407	THR
1	C	411	LEU
1	C	416	ARG
1	C	429	VAL
1	C	441	GLN
1	C	443	MET
1	D	47	VAL
1	D	127	ILE
1	D	306	ILE
1	D	324	LEU
1	D	332	ILE
1	D	333	THR
1	D	336	ARG
1	D	338	THR
1	D	350	LEU
1	D	378	GLU
1	D	382	MET
1	D	390	LEU
1	D	407	THR
1	D	429	VAL
1	D	441	GLN
1	E	127	ILE

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Mol	Chain	Res	Type
1	E	306	ILE
1	E	324	LEU
1	E	332	ILE
1	E	333	THR
1	E	338	THR
1	E	350	LEU
1	E	378	GLU
1	E	381	GLU
1	E	382	MET
1	E	384	GLU
1	E	390	LEU
1	E	407	THR
1	E	429	VAL
1	E	441	GLN
1	F	47	VAL
1	F	306	ILE
1	F	324	LEU
1	F	332	ILE
1	F	333	THR
1	F	336	ARG
1	F	338	THR
1	F	350	LEU
1	F	378	GLU
1	F	382	MET
1	F	390	LEU
1	F	407	THR
1	F	411	LEU
1	F	429	VAL
1	F	441	GLN
1	F	450	PHE
1	F	451	LEU
1	G	15	ASP
1	G	19	ILE
1	G	46	MET
1	G	47	VAL
1	G	127	ILE
1	G	306	ILE
1	G	324	LEU
1	G	332	ILE
1	G	333	THR
1	G	338	THR
1	G	350	LEU

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Mol	Chain	Res	Type
1	G	378	GLU
1	G	382	MET
1	G	390	LEU
1	G	407	THR
1	G	411	LEU
1	G	416	ARG
1	G	429	VAL
1	G	443	MET
1	H	47	VAL
1	H	332	ILE
1	H	333	THR
1	H	338	THR
1	H	378	GLU
1	H	390	LEU
1	H	407	THR
1	H	410	SER
1	H	411	LEU
1	H	429	VAL
1	H	441	GLN
1	I	47	VAL
1	I	127	ILE
1	I	267	GLU
1	I	306	ILE
1	I	324	LEU
1	I	333	THR
1	I	338	THR
1	I	382	MET
1	I	390	LEU
1	I	407	THR
1	I	429	VAL
1	I	443	MET
1	J	260	LEU
1	J	306	ILE
1	J	332	ILE
1	J	333	THR
1	J	336	ARG
1	J	338	THR
1	J	350	LEU
1	J	407	THR
1	J	429	VAL
1	J	441	GLN
1	K	40	ARG

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Mol	Chain	Res	Type
1	K	46	MET
1	K	127	ILE
1	K	324	LEU
1	K	333	THR
1	K	338	THR
1	K	350	LEU
1	K	390	LEU
1	K	407	THR
1	K	429	VAL
1	L	285	GLU
1	L	306	ILE
1	L	332	ILE
1	L	333	THR
1	L	338	THR
1	L	350	LEU
1	L	429	VAL
1	L	443	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	302	HIS
1	A	313	ASN
1	B	49	GLN
1	B	302	HIS
1	B	313	ASN
1	C	49	GLN
1	C	302	HIS
1	C	313	ASN
1	D	49	GLN
1	D	302	HIS
1	D	313	ASN
1	E	49	GLN
1	E	302	HIS
1	E	313	ASN
1	F	49	GLN
1	F	302	HIS
1	F	313	ASN
1	F	369	GLN
1	G	302	HIS
1	G	313	ASN

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Mol	Chain	Res	Type
1	G	369	GLN
1	H	302	HIS
1	H	313	ASN
1	I	302	HIS
1	J	92	GLN
1	J	302	HIS
1	J	313	ASN
1	K	49	GLN
1	K	313	ASN
1	L	302	HIS
1	L	313	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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	I	1450	-	28,29,29	0.34	0	43,45,45	0.54	0
2	ADP	B	1450	-	28,29,29	0.35	0	43,45,45	0.56	0
2	ADP	G	1450	-	28,29,29	0.33	0	43,45,45	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ADP	C	1450	-	28,29,29	0.55	1 (3%)	43,45,45	0.51	0
2	ADP	D	1450	-	28,29,29	0.30	0	43,45,45	0.53	0
2	ADP	J	1450	-	28,29,29	0.38	0	43,45,45	0.53	0
2	ADP	F	1450	-	28,29,29	0.36	0	43,45,45	0.60	0
2	ADP	H	1450	-	28,29,29	0.46	0	43,45,45	0.52	0
2	ADP	L	1450	-	28,29,29	0.30	0	43,45,45	0.52	0
2	ADP	A	1450	-	28,29,29	0.35	0	43,45,45	0.55	0
2	ADP	E	1450	-	28,29,29	0.34	0	43,45,45	0.65	1 (2%)
2	ADP	K	1450	-	22,26,29	0.39	0	33,38,45	0.59	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	I	1450	-	-	4/16/32/32	0/3/3/3
2	ADP	B	1450	-	-	3/16/32/32	0/3/3/3
2	ADP	G	1450	-	-	4/16/32/32	0/3/3/3
2	ADP	C	1450	-	-	3/16/32/32	0/3/3/3
2	ADP	D	1450	-	-	5/16/32/32	0/3/3/3
2	ADP	J	1450	-	-	6/16/32/32	0/3/3/3
2	ADP	F	1450	-	-	4/16/32/32	0/3/3/3
2	ADP	H	1450	-	-	3/16/32/32	0/3/3/3
2	ADP	L	1450	-	-	3/16/32/32	0/3/3/3
2	ADP	A	1450	-	-	3/16/32/32	0/3/3/3
2	ADP	E	1450	-	-	3/16/32/32	0/3/3/3
2	ADP	K	1450	-	-	0/6/22/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1450	ADP	PB-O1B	2.20	1.57	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1450	ADP	O2'-C2'-C1'	2.14	117.47	110.10

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1450	ADP	C5'-O5'-PA-O1A
2	A	1450	ADP	C5'-O5'-PA-O2A
2	A	1450	ADP	C5'-O5'-PA-O3A
2	B	1450	ADP	C5'-O5'-PA-O1A
2	B	1450	ADP	C5'-O5'-PA-O2A
2	B	1450	ADP	C5'-O5'-PA-O3A
2	C	1450	ADP	C5'-O5'-PA-O1A
2	C	1450	ADP	C5'-O5'-PA-O2A
2	C	1450	ADP	C5'-O5'-PA-O3A
2	D	1450	ADP	C5'-O5'-PA-O1A
2	D	1450	ADP	C5'-O5'-PA-O2A
2	D	1450	ADP	C5'-O5'-PA-O3A
2	E	1450	ADP	C5'-O5'-PA-O1A
2	E	1450	ADP	C5'-O5'-PA-O2A
2	E	1450	ADP	C5'-O5'-PA-O3A
2	F	1450	ADP	C5'-O5'-PA-O1A
2	F	1450	ADP	C5'-O5'-PA-O2A
2	F	1450	ADP	C5'-O5'-PA-O3A
2	G	1450	ADP	C5'-O5'-PA-O1A
2	G	1450	ADP	C5'-O5'-PA-O2A
2	G	1450	ADP	C5'-O5'-PA-O3A
2	H	1450	ADP	C5'-O5'-PA-O2A
2	H	1450	ADP	C5'-O5'-PA-O3A
2	I	1450	ADP	C5'-O5'-PA-O1A
2	I	1450	ADP	C5'-O5'-PA-O2A
2	I	1450	ADP	C5'-O5'-PA-O3A
2	J	1450	ADP	PA-O3A-PB-O3B
2	J	1450	ADP	C5'-O5'-PA-O2A
2	L	1450	ADP	C5'-O5'-PA-O1A
2	L	1450	ADP	C5'-O5'-PA-O2A
2	L	1450	ADP	C5'-O5'-PA-O3A
2	J	1450	ADP	PA-O3A-PB-O2B
2	H	1450	ADP	C5'-O5'-PA-O1A
2	J	1450	ADP	C5'-O5'-PA-O1A
2	J	1450	ADP	C5'-O5'-PA-O3A
2	F	1450	ADP	PB-O3A-PA-O2A
2	J	1450	ADP	PA-O3A-PB-O1B
2	D	1450	ADP	PB-O3A-PA-O2A
2	G	1450	ADP	PB-O3A-PA-O2A
2	D	1450	ADP	PB-O3A-PA-O1A

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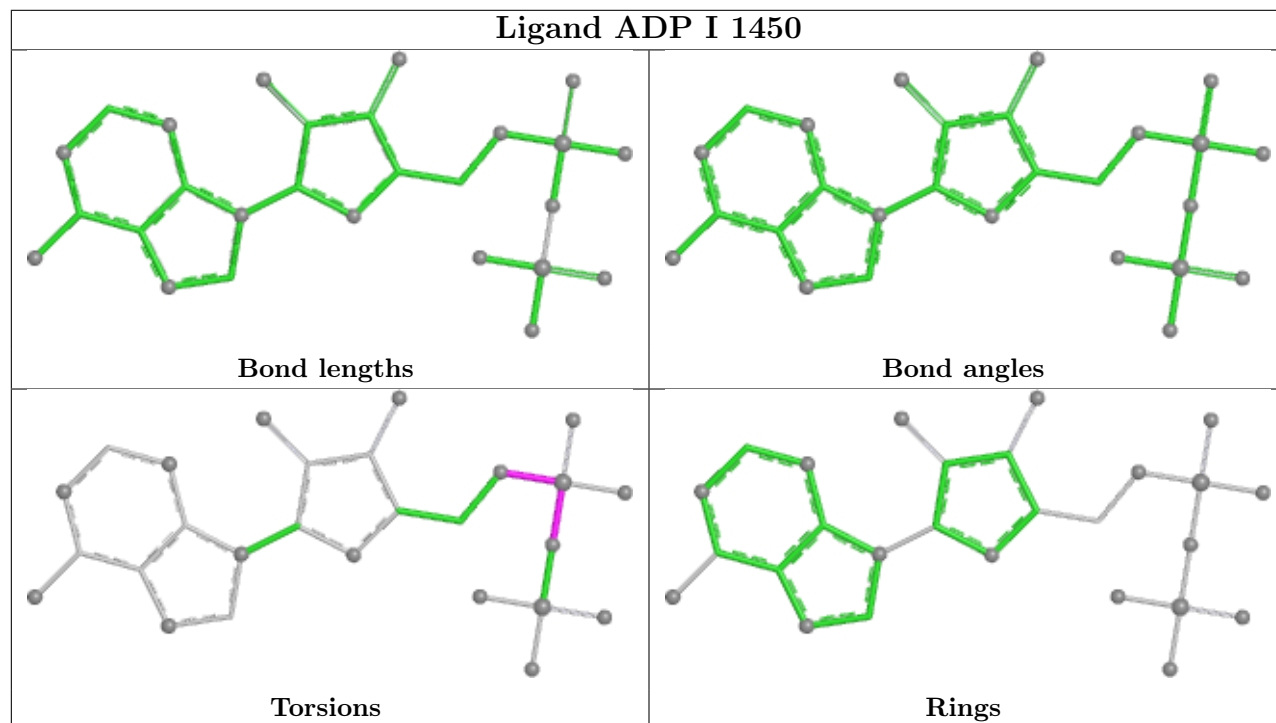
Mol	Chain	Res	Type	Atoms
2	I	1450	ADP	PB-O3A-PA-O2A

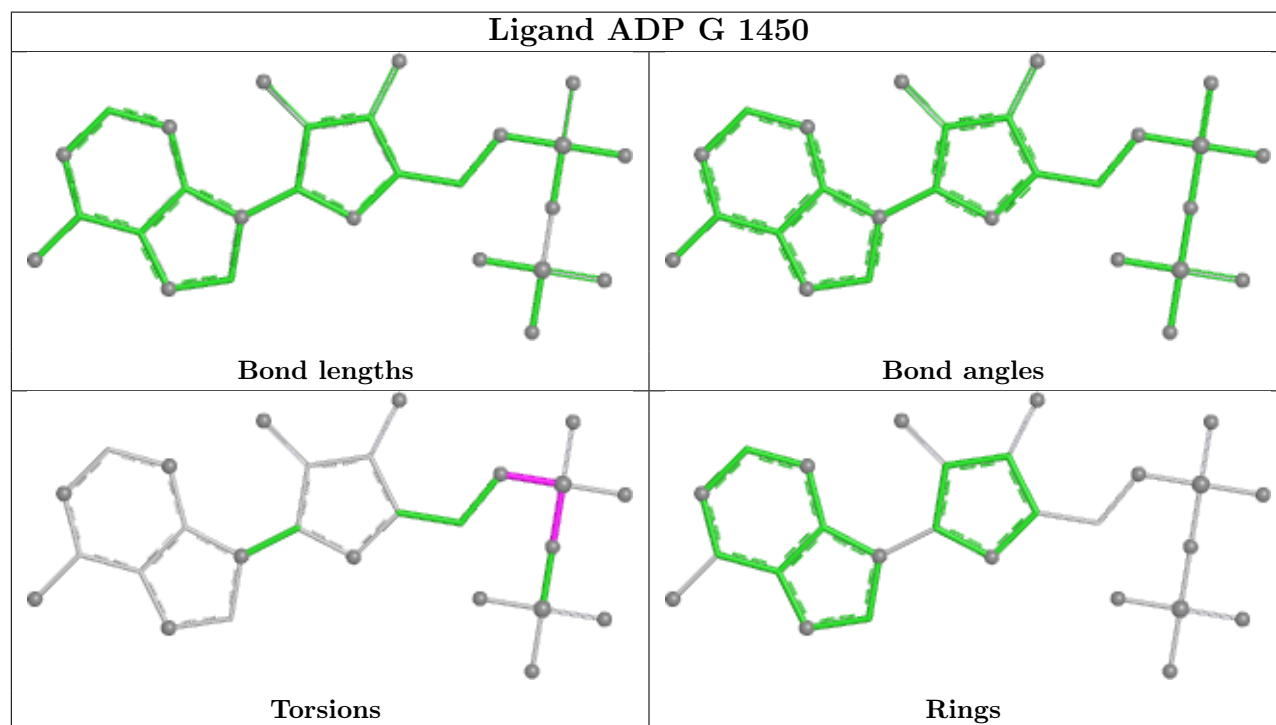
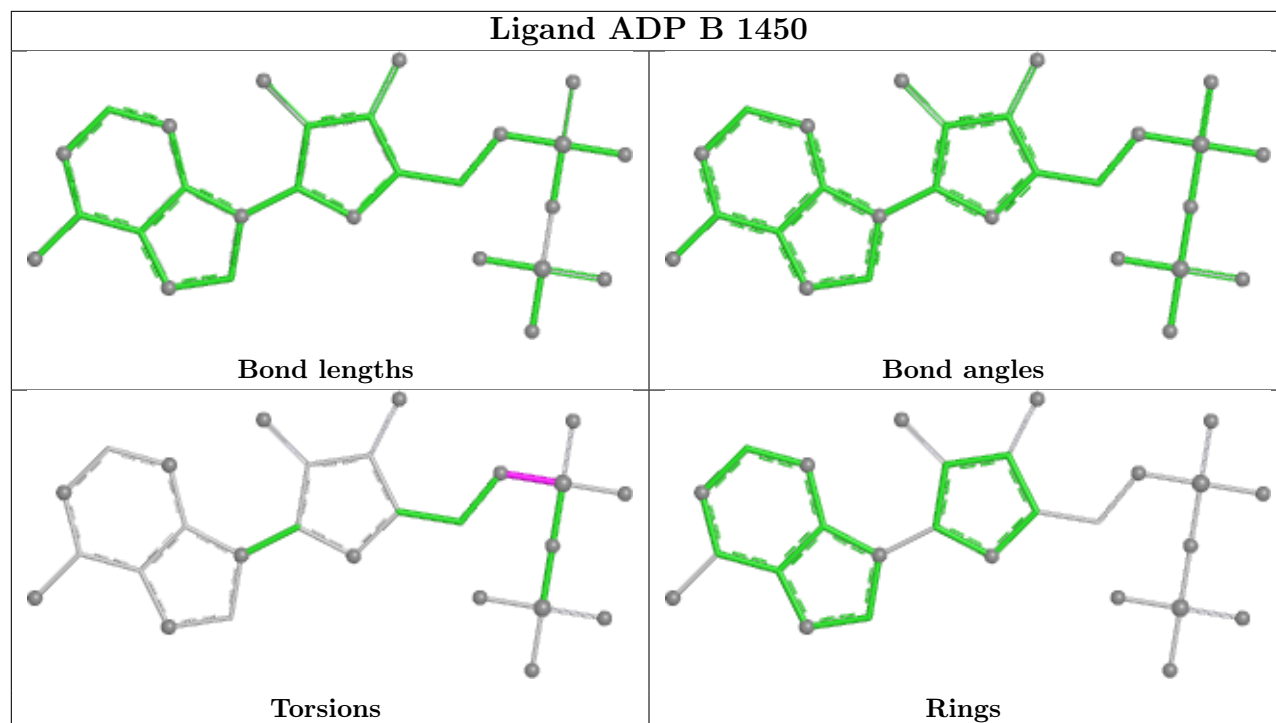
There are no ring outliers.

1 monomer is involved in 1 short contact:

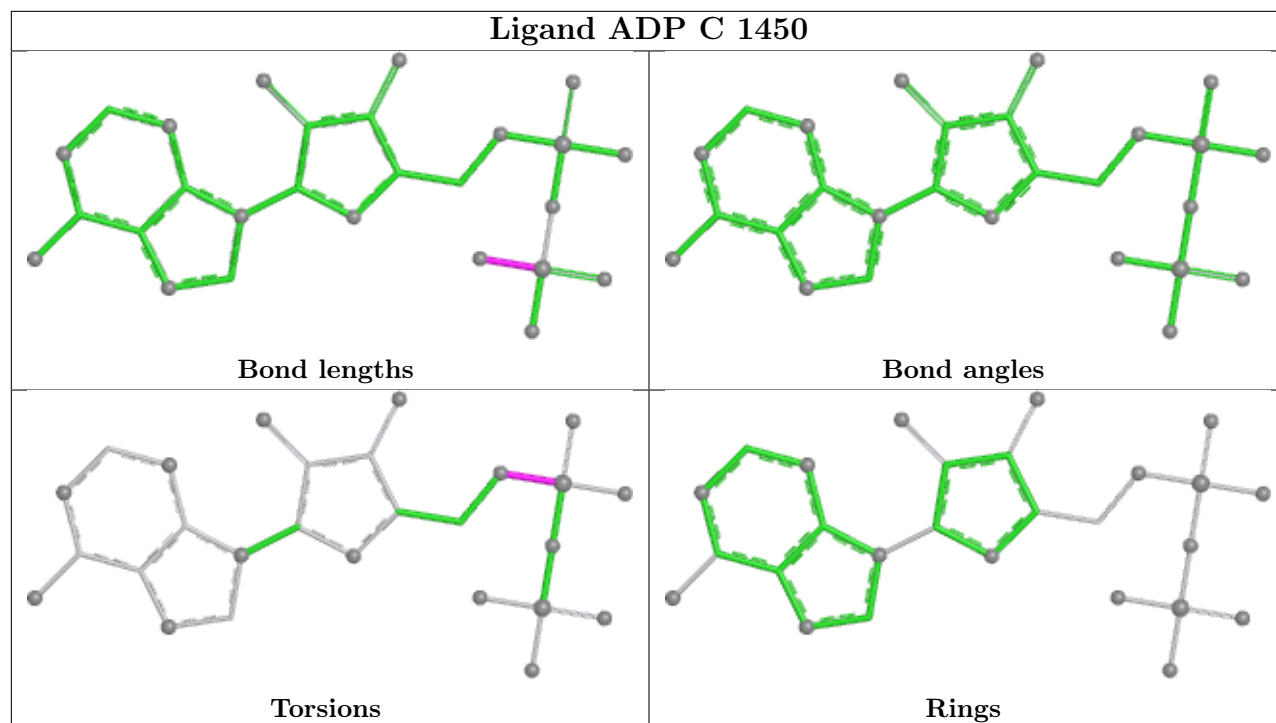
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1450	ADP	1	0

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.

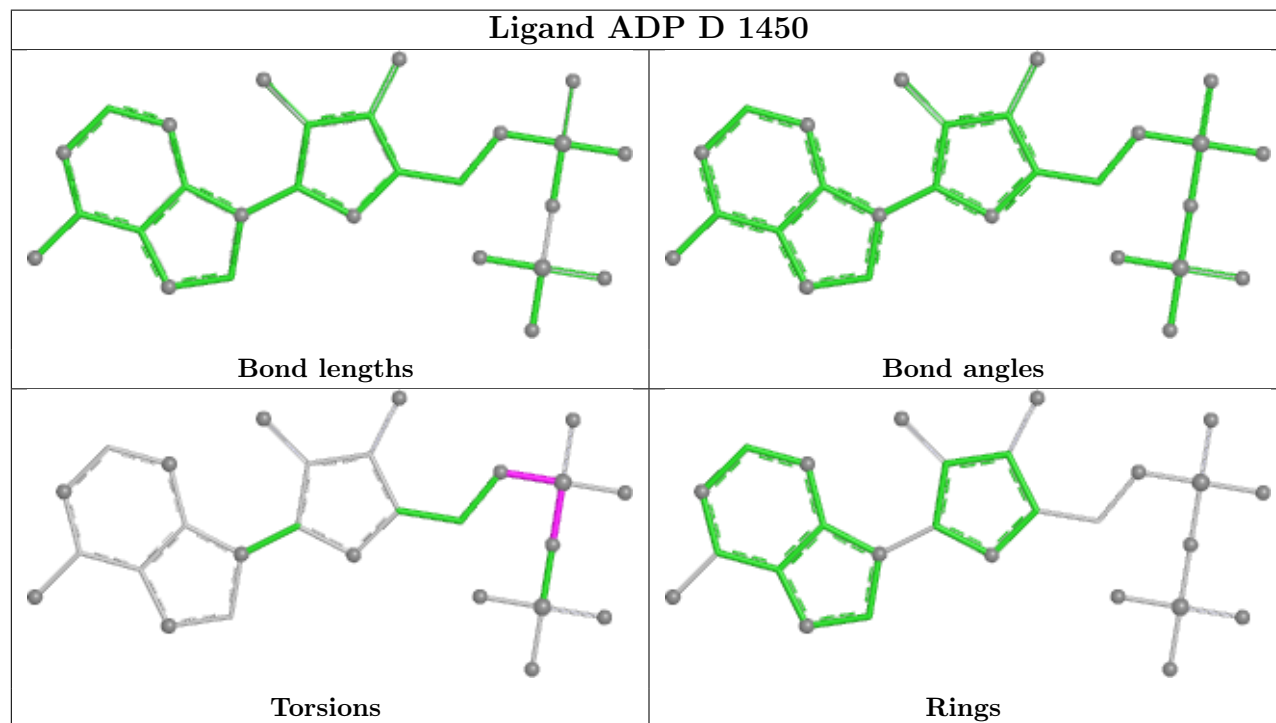


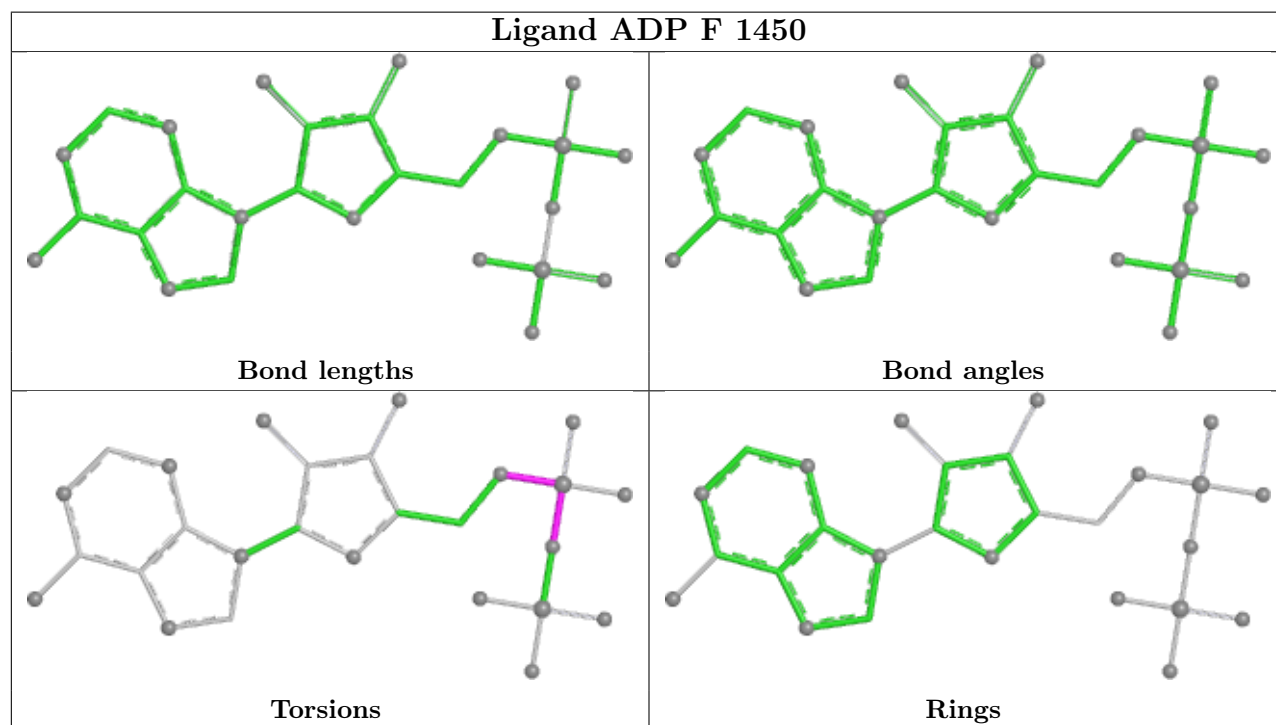
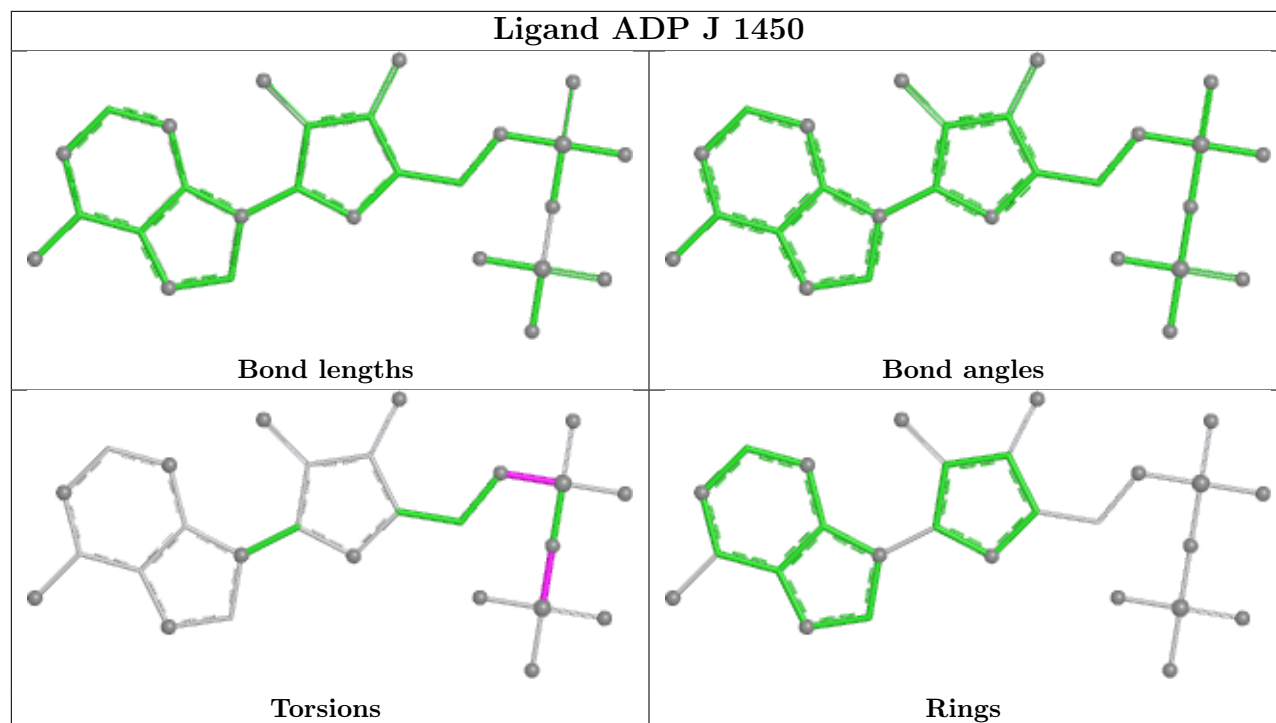


Ligand ADP C 1450

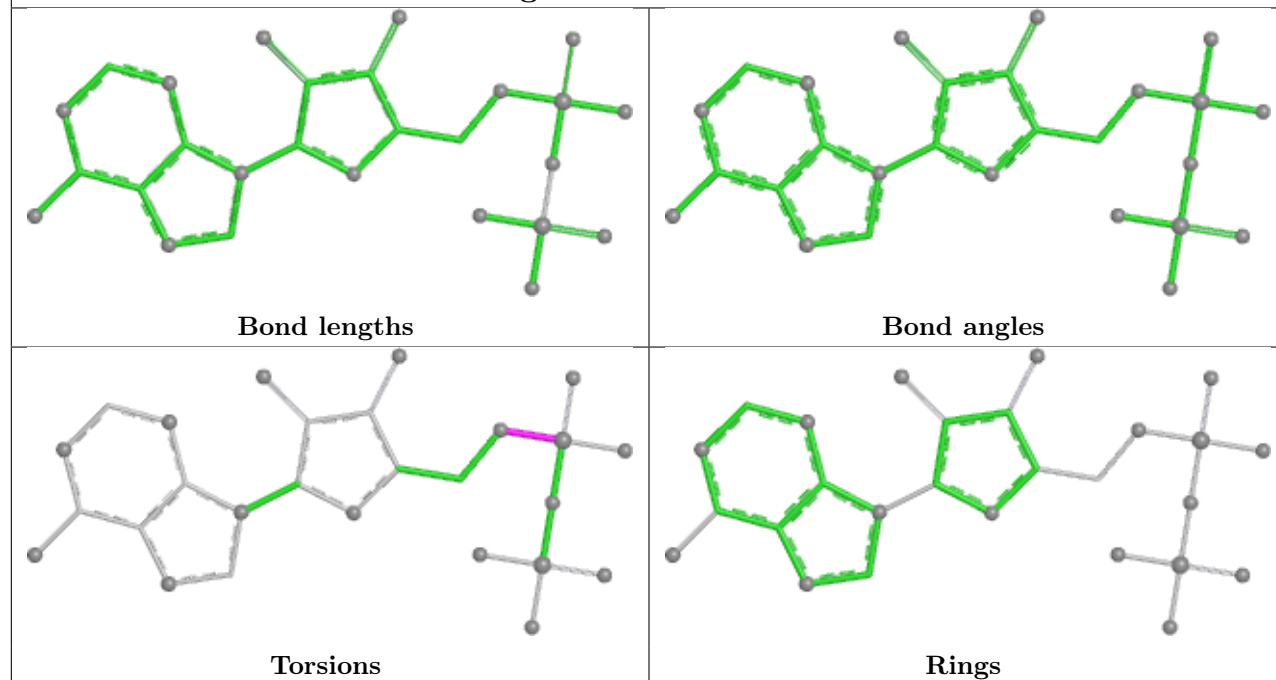


Ligand ADP D 1450

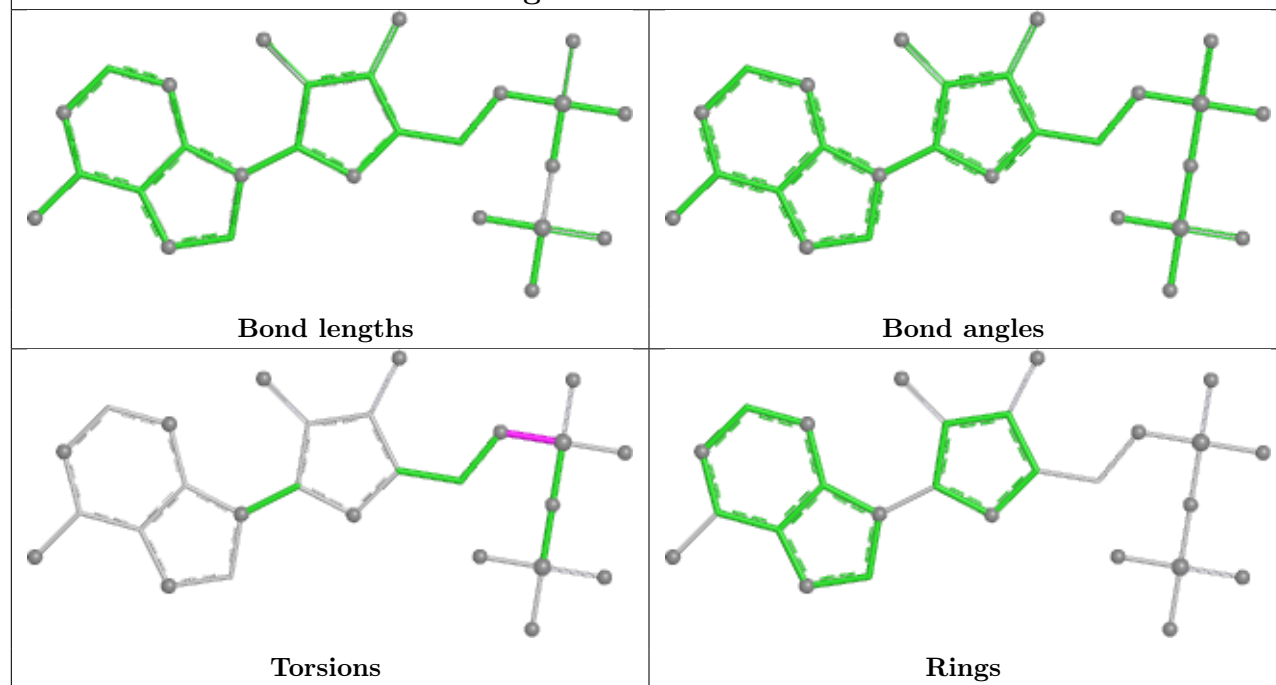


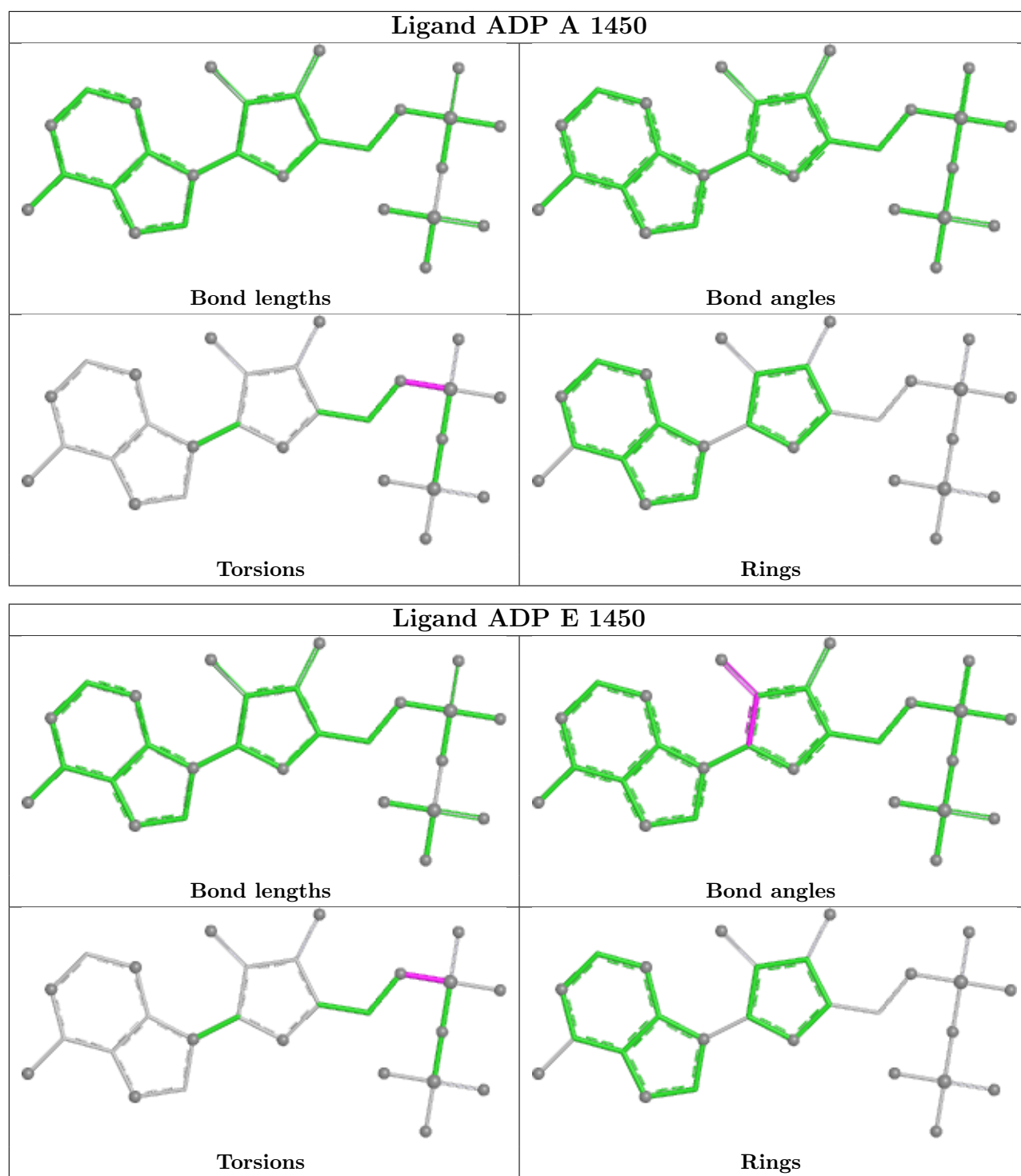


Ligand ADP H 1450



Ligand ADP L 1450





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	298/368 (80%)	0.70	21 (7%) 22 19	53, 87, 127, 149	0
1	B	300/368 (81%)	0.58	27 (9%) 15 13	46, 82, 118, 137	0
1	C	321/368 (87%)	0.39	15 (4%) 36 30	46, 76, 104, 125	0
1	D	299/368 (81%)	0.69	26 (8%) 16 14	57, 90, 125, 143	0
1	E	290/368 (78%)	0.68	23 (7%) 18 16	49, 85, 140, 170	0
1	F	301/368 (81%)	0.57	21 (6%) 22 19	43, 77, 114, 147	0
1	G	330/368 (89%)	0.44	18 (5%) 30 25	46, 81, 121, 146	0
1	H	277/368 (75%)	1.04	38 (13%) 6 6	73, 112, 148, 173	0
1	I	294/368 (79%)	1.14	58 (19%) 3 3	58, 106, 139, 154	0
1	J	300/368 (81%)	1.01	43 (14%) 6 6	61, 105, 136, 155	0
1	K	283/368 (76%)	1.59	90 (31%) 1 1	75, 95, 117, 159	0
1	L	233/368 (63%)	1.44	61 (26%) 1 1	69, 123, 170, 185	0
All	All	3526/4416 (79%)	0.83	441 (12%) 8 7	43, 92, 137, 185	0

All (441) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	402	ALA	6.4
1	H	79	PRO	5.7
1	I	422	GLN	5.5
1	I	420	GLU	5.5
1	K	43	SER	5.4
1	L	425	ASP	5.2
1	I	360	THR	5.1
1	L	125	ARG	5.1
1	K	47	VAL	4.9
1	F	443	MET	4.8
1	J	416	ARG	4.7

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Mol	Chain	Res	Type	RSRZ
1	J	31	LEU	4.7
1	B	42	ALA	4.7
1	H	352	ASP	4.6
1	I	31	LEU	4.5
1	J	442	TYR	4.5
1	L	321	ALA	4.4
1	K	86	ILE	4.4
1	K	402	ALA	4.3
1	L	391	THR	4.3
1	L	245	HIS	4.3
1	E	93	ALA	4.3
1	H	276	ILE	4.2
1	G	419	THR	4.2
1	I	251	ASN	4.2
1	K	106	SER	4.1
1	I	362	TYR	4.1
1	K	45	GLY	4.0
1	E	409	ALA	4.0
1	K	371	LEU	3.9
1	I	412	VAL	3.9
1	J	22	ILE	3.9
1	K	89	GLY	3.9
1	F	251	ASN	3.8
1	B	259	ALA	3.8
1	K	399	LEU	3.8
1	I	389	VAL	3.8
1	L	410	SER	3.8
1	C	251	ASN	3.8
1	I	263	GLY	3.8
1	K	276	ILE	3.7
1	K	298	ILE	3.7
1	K	426	ILE	3.7
1	L	250	ILE	3.7
1	K	394	GLY	3.7
1	L	123	PHE	3.7
1	B	40	ARG	3.6
1	G	426	ILE	3.6
1	F	284	ARG	3.5
1	L	363	SER	3.5
1	K	391	THR	3.5
1	G	337	GLY	3.5
1	I	384	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	106	SER	3.5
1	K	253	ARG	3.5
1	K	51	ALA	3.5
1	E	90	MET	3.4
1	K	381	GLU	3.4
1	A	410	SER	3.4
1	A	28	ILE	3.4
1	J	396	GLU	3.4
1	K	413	CYS	3.4
1	H	52	ALA	3.4
1	I	93	ALA	3.4
1	L	431	SER	3.4
1	J	46	MET	3.4
1	D	426	ILE	3.4
1	D	424	ASP	3.4
1	L	435	ASP	3.4
1	J	17	THR	3.3
1	K	378	GLU	3.3
1	B	426	ILE	3.3
1	J	337	GLY	3.3
1	J	19	ILE	3.3
1	K	373	ILE	3.3
1	L	243	SER	3.3
1	D	131	ILE	3.3
1	C	241	THR	3.3
1	B	112	GLU	3.2
1	K	119	LEU	3.2
1	L	404	GLN	3.2
1	E	105	GLY	3.2
1	J	402	ALA	3.2
1	I	397	THR	3.2
1	J	379	ASP	3.2
1	L	101	THR	3.2
1	K	90	MET	3.2
1	I	36	ALA	3.2
1	D	44	GLN	3.2
1	K	403	ILE	3.2
1	I	385	ASP	3.1
1	H	129	VAL	3.1
1	K	370	ILE	3.1
1	A	252	SER	3.1
1	C	19	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	I	76	ALA	3.1
1	K	118	ALA	3.1
1	A	257	PHE	3.1
1	L	129	VAL	3.1
1	B	349	ASP	3.1
1	B	260	LEU	3.1
1	L	399	LEU	3.1
1	H	102	ALA	3.0
1	I	421	VAL	3.0
1	H	262	SER	3.0
1	E	94	LEU	3.0
1	F	444	LYS	3.0
1	L	37	LEU	3.0
1	H	391	THR	3.0
1	L	76	ALA	3.0
1	H	252	SER	3.0
1	H	45	GLY	3.0
1	J	369	GLN	3.0
1	L	375	CYS	3.0
1	J	244	LEU	3.0
1	H	421	VAL	3.0
1	J	16	VAL	3.0
1	L	411	LEU	3.0
1	K	91	ALA	3.0
1	K	367	THR	3.0
1	D	280	VAL	3.0
1	I	380	VAL	3.0
1	F	283	TRP	2.9
1	H	71	ARG	2.9
1	A	426	ILE	2.9
1	D	352	ASP	2.9
1	K	313	ASN	2.9
1	I	431	SER	2.9
1	J	268	ILE	2.9
1	L	275	GLN	2.9
1	K	320	MET	2.9
1	I	399	LEU	2.9
1	K	324	LEU	2.9
1	J	283	TRP	2.9
1	K	436	GLU	2.9
1	K	363	SER	2.9
1	I	280	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	L	428	ARG	2.9
1	I	418	GLY	2.9
1	F	446	TYR	2.9
1	K	101	THR	2.9
1	L	81	THR	2.9
1	H	28	ILE	2.9
1	L	442	TYR	2.8
1	J	68	ILE	2.8
1	A	288	LYS	2.8
1	K	27	HIS	2.8
1	L	436	GLU	2.8
1	J	430	TYR	2.8
1	K	380	VAL	2.8
1	K	321	ALA	2.8
1	D	70	GLY	2.8
1	F	80	GLY	2.8
1	K	280	VAL	2.8
1	K	362	TYR	2.8
1	C	426	ILE	2.8
1	D	68	ILE	2.8
1	D	248	ASP	2.8
1	G	443	MET	2.8
1	I	262	SER	2.8
1	K	345	GLY	2.8
1	L	295	VAL	2.7
1	A	292	ILE	2.7
1	H	371	LEU	2.7
1	I	419	THR	2.7
1	K	397	THR	2.7
1	B	263	GLY	2.7
1	D	291	ILE	2.7
1	K	325	ILE	2.7
1	K	351	LEU	2.7
1	K	415	LYS	2.7
1	L	77	GLY	2.7
1	B	111	LEU	2.7
1	J	370	ILE	2.7
1	L	109	PHE	2.7
1	F	387	TYR	2.7
1	I	277	ASN	2.7
1	I	54	ARG	2.7
1	E	366	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	349	ASP	2.7
1	K	319	ASP	2.7
1	J	43	SER	2.7
1	K	304	LEU	2.7
1	E	402	ALA	2.7
1	A	48	GLY	2.7
1	B	394	GLY	2.7
1	C	422	GLN	2.7
1	D	341	GLN	2.7
1	E	272	VAL	2.7
1	K	272	VAL	2.7
1	D	63	ILE	2.6
1	L	351	LEU	2.7
1	L	329	ASN	2.6
1	B	406	ILE	2.6
1	K	335	ILE	2.6
1	D	42	ALA	2.6
1	D	410	SER	2.6
1	K	32	GLY	2.6
1	J	338	THR	2.6
1	K	422	GLN	2.6
1	B	379	ASP	2.6
1	K	104	ALA	2.6
1	F	437	SER	2.6
1	H	390	LEU	2.6
1	I	367	THR	2.6
1	I	423	VAL	2.6
1	L	405	LEU	2.6
1	K	113	MET	2.6
1	I	425	ASP	2.6
1	K	318	SER	2.6
1	L	283	TRP	2.6
1	J	254	THR	2.6
1	K	306	ILE	2.6
1	K	326	MET	2.6
1	K	333	THR	2.6
1	L	424	ASP	2.6
1	G	387	TYR	2.5
1	K	434	LEU	2.5
1	I	325	ILE	2.5
1	L	249	VAL	2.5
1	L	412	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	251	ASN	2.5
1	E	97	ASP	2.5
1	L	432	LEU	2.5
1	B	393	ILE	2.5
1	L	254	THR	2.5
1	J	76	ALA	2.5
1	B	352	ASP	2.5
1	L	279	LYS	2.5
1	I	426	ILE	2.5
1	H	387	TYR	2.5
1	G	307	GLU	2.5
1	H	78	GLN	2.5
1	L	315	ALA	2.5
1	L	359	THR	2.5
1	D	40	ARG	2.5
1	L	248	ASP	2.5
1	B	258	LEU	2.5
1	B	316	LEU	2.5
1	F	399	LEU	2.5
1	H	348	ILE	2.5
1	L	383	SER	2.5
1	A	412	VAL	2.5
1	I	430	TYR	2.5
1	K	307	GLU	2.5
1	F	116	THR	2.5
1	I	69	ALA	2.5
1	L	374	ARG	2.5
1	A	393	ILE	2.4
1	K	393	ILE	2.4
1	K	297	PHE	2.4
1	K	374	ARG	2.4
1	K	275	GLN	2.4
1	I	37	LEU	2.4
1	I	46	MET	2.4
1	J	276	ILE	2.4
1	A	80	GLY	2.4
1	I	372	ARG	2.4
1	L	124	ARG	2.4
1	H	38	GLU	2.4
1	D	281	ALA	2.4
1	E	278	ALA	2.4
1	G	259	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	247	ILE	2.4
1	L	393	ILE	2.4
1	I	357	VAL	2.4
1	L	429	VAL	2.4
1	E	318	SER	2.4
1	C	419	THR	2.4
1	I	432	LEU	2.4
1	H	361	PRO	2.4
1	D	30	GLY	2.4
1	H	47	VAL	2.4
1	L	421	VAL	2.4
1	K	97	ASP	2.4
1	E	271	GLU	2.4
1	L	112	GLU	2.4
1	G	289	ALA	2.4
1	F	41	GLN	2.4
1	K	26	SER	2.4
1	H	283	TRP	2.4
1	H	320	MET	2.4
1	I	401	TYR	2.4
1	B	131	ILE	2.4
1	L	276	ILE	2.4
1	L	426	ILE	2.4
1	J	361	PRO	2.4
1	K	293	PRO	2.4
1	B	280	VAL	2.3
1	C	337	GLY	2.3
1	F	29	ARG	2.3
1	K	70	GLY	2.3
1	E	379	ASP	2.3
1	K	379	ASP	2.3
1	K	300	GLU	2.3
1	L	107	GLU	2.3
1	A	358	SER	2.3
1	A	68	ILE	2.3
1	A	370	ILE	2.3
1	H	63	ILE	2.3
1	I	298	ILE	2.3
1	C	45	GLY	2.3
1	K	251	ASN	2.3
1	E	443	MET	2.3
1	D	434	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	308	SER	2.3
1	K	308	SER	2.3
1	B	68	ILE	2.3
1	G	406	ILE	2.3
1	H	362	TYR	2.3
1	L	284	ARG	2.3
1	K	433	PHE	2.3
1	I	24	ALA	2.3
1	J	409	ALA	2.3
1	H	46	MET	2.3
1	K	305	ASP	2.3
1	J	49	GLN	2.3
1	I	407	THR	2.3
1	K	98	THR	2.3
1	K	82	GLY	2.3
1	C	259	ALA	2.3
1	D	320	MET	2.3
1	D	319	ASP	2.3
1	F	349	ASP	2.3
1	J	349	ASP	2.3
1	B	413	CYS	2.3
1	J	8	THR	2.3
1	C	46	MET	2.2
1	G	386	ALA	2.2
1	C	108	ILE	2.2
1	H	273	ARG	2.2
1	K	347	PRO	2.2
1	A	320	MET	2.2
1	G	258	LEU	2.2
1	D	97	ASP	2.2
1	I	379	ASP	2.2
1	D	375	CYS	2.2
1	L	106	SER	2.2
1	K	77	GLY	2.2
1	F	320	MET	2.2
1	H	88	MET	2.2
1	K	24	ALA	2.2
1	F	393	ILE	2.2
1	I	247	ILE	2.2
1	I	374	ARG	2.2
1	J	291	ILE	2.2
1	L	325	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	413	CYS	2.2
1	F	337	GLY	2.2
1	I	382	MET	2.2
1	I	383	SER	2.2
1	I	398	SER	2.2
1	E	433	PHE	2.2
1	I	436	GLU	2.2
1	D	268	ILE	2.2
1	K	346	ILE	2.2
1	G	422	GLN	2.2
1	J	277	ASN	2.2
1	F	417	LYS	2.2
1	J	365	LYS	2.2
1	C	250	ILE	2.1
1	F	130	ARG	2.1
1	H	292	ILE	2.1
1	J	284	ARG	2.1
1	H	347	PRO	2.1
1	K	84	THR	2.1
1	A	244	LEU	2.1
1	H	123	PHE	2.1
1	K	354	LEU	2.1
1	B	330	ARG	2.1
1	D	53	ARG	2.1
1	F	420	GLU	2.1
1	J	20	GLU	2.1
1	E	341	GLN	2.1
1	B	277	ASN	2.1
1	L	272	VAL	2.1
1	K	368	LYS	2.1
1	G	349	ASP	2.1
1	A	419	THR	2.1
1	I	23	GLY	2.1
1	I	371	LEU	2.1
1	C	386	ALA	2.1
1	I	85	ALA	2.1
1	J	387	TYR	2.1
1	K	442	TYR	2.1
1	B	276	ILE	2.1
1	K	383	SER	2.1
1	E	313	ASN	2.1
1	H	423	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	89	GLY	2.1
1	H	316	LEU	2.1
1	A	387	TYR	2.1
1	C	291	ILE	2.1
1	K	310	SER	2.1
1	G	320	MET	2.1
1	J	27	HIS	2.1
1	K	301	VAL	2.1
1	B	37	LEU	2.1
1	E	432	LEU	2.1
1	J	434	LEU	2.1
1	A	287	GLY	2.1
1	L	433	PHE	2.1
1	E	352	ASP	2.1
1	F	69	ALA	2.1
1	I	408	ALA	2.1
1	J	103	ILE	2.1
1	K	63	ILE	2.1
1	L	267	GLU	2.1
1	D	46	MET	2.0
1	K	126	SER	2.0
1	E	41	GLN	2.0
1	L	365	LYS	2.0
1	I	27	HIS	2.0
1	I	429	VAL	2.0
1	L	280	VAL	2.0
1	G	96	PRO	2.0
1	L	322	PRO	2.0
1	A	372	ARG	2.0
1	B	80	GLY	2.0
1	G	253	ARG	2.0
1	I	287	GLY	2.0
1	J	433	PHE	2.0
1	B	265	THR	2.0
1	C	349	ASP	2.0
1	E	426	ILE	2.0
1	H	406	ILE	2.0
1	J	327	ALA	2.0
1	G	47	VAL	2.0
1	H	280	VAL	2.0
1	I	43	SER	2.0
1	J	252	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	K	342	SER	2.0
1	G	39	PRO	2.0
1	I	347	PRO	2.0
1	E	40	ARG	2.0
1	K	71	ARG	2.0
1	J	100	PHE	2.0
1	K	105	GLY	2.0
1	K	407	THR	2.0
1	I	73	VAL	2.0
1	J	301	VAL	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](#)

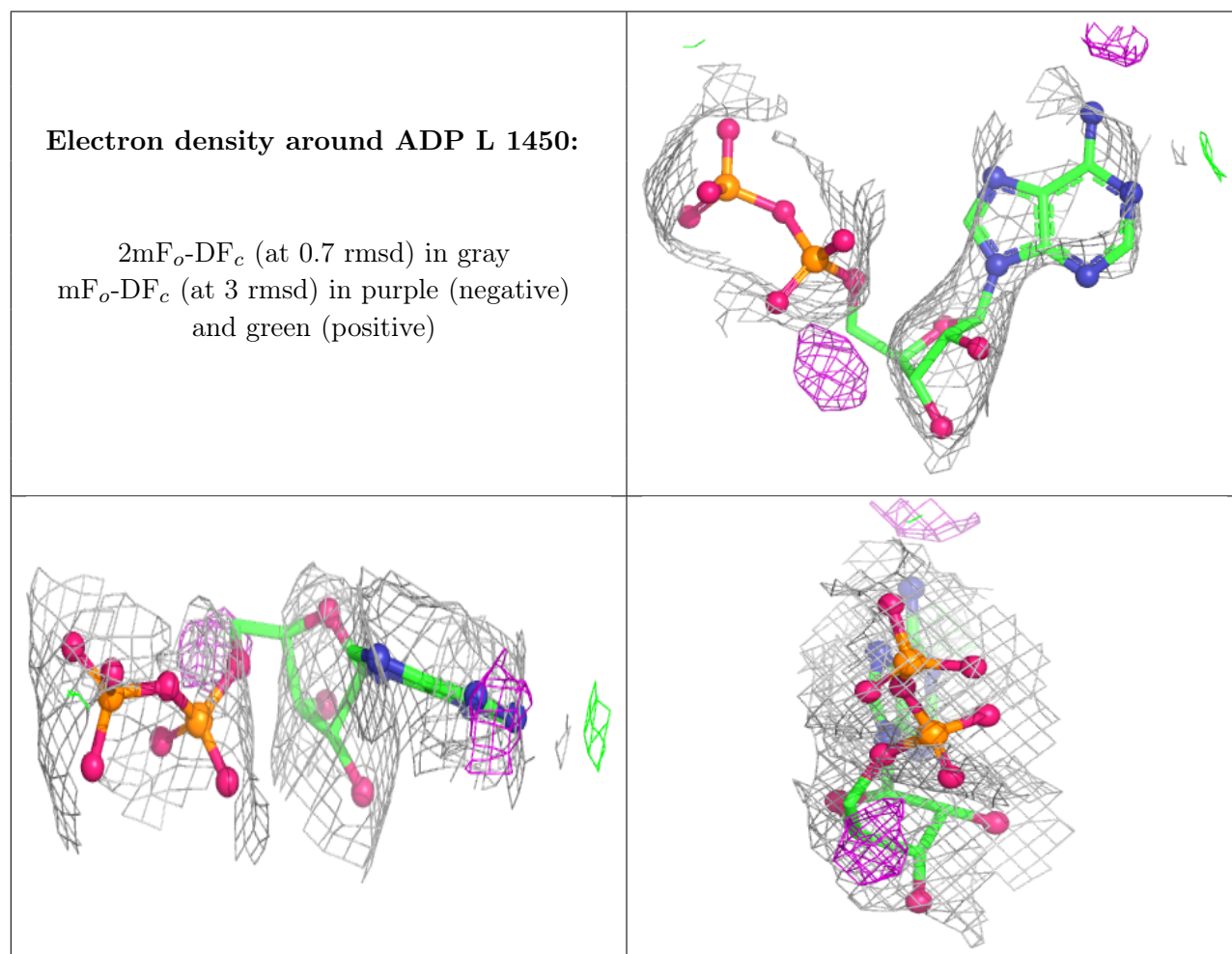
There are no oligosaccharides in this entry.

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.

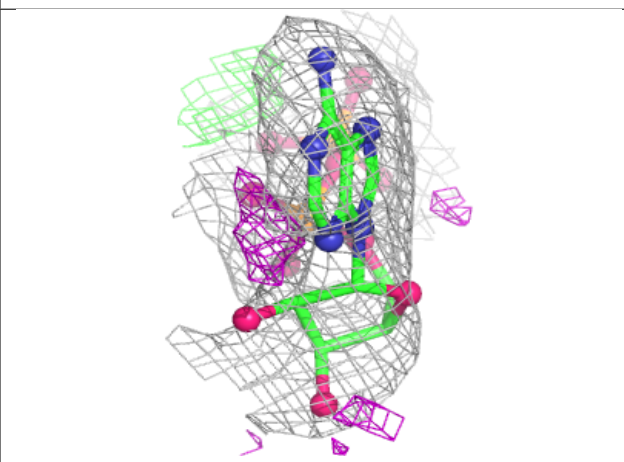
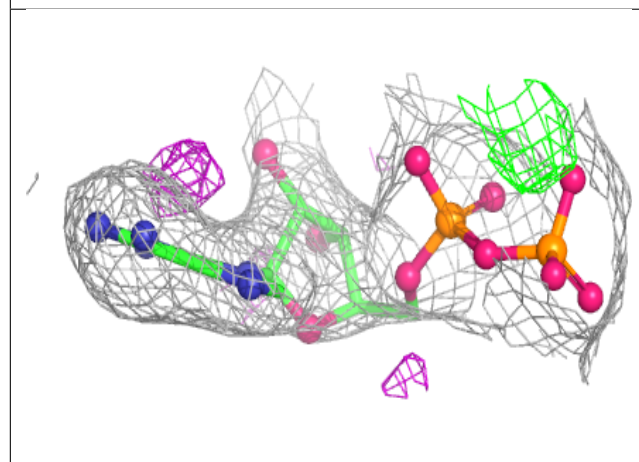
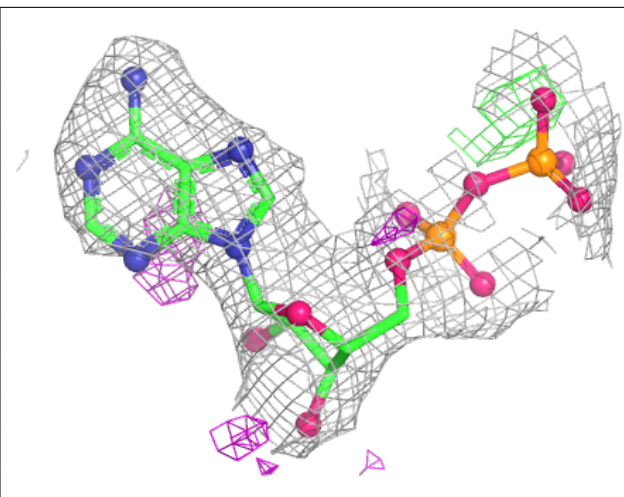
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ADP	K	1450	25/27	0.71	0.15	79,90,94,98	0
2	ADP	L	1450	27/27	0.86	0.13	117,125,133,135	0
2	ADP	I	1450	27/27	0.88	0.13	110,126,135,137	0
2	ADP	H	1450	27/27	0.94	0.11	94,102,116,118	0
2	ADP	F	1450	27/27	0.94	0.09	65,71,84,86	0
2	ADP	C	1450	27/27	0.95	0.09	66,74,80,82	0
2	ADP	J	1450	27/27	0.95	0.09	92,113,131,133	0
2	ADP	D	1450	27/27	0.96	0.09	73,78,94,101	0
2	ADP	E	1450	27/27	0.96	0.09	74,83,88,89	0
2	ADP	B	1450	27/27	0.96	0.08	58,70,81,83	0
2	ADP	A	1450	27/27	0.96	0.08	73,78,83,84	0
2	ADP	G	1450	27/27	0.97	0.07	59,68,75,77	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.



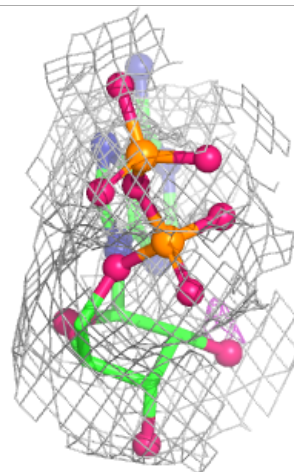
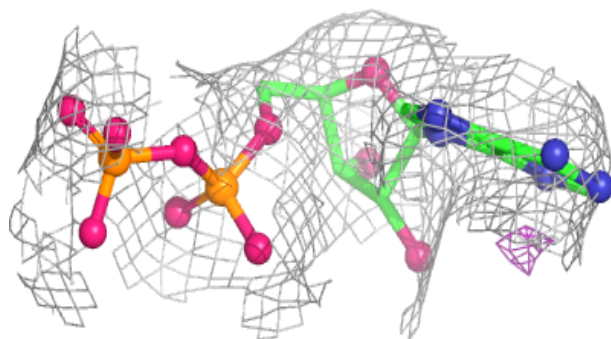
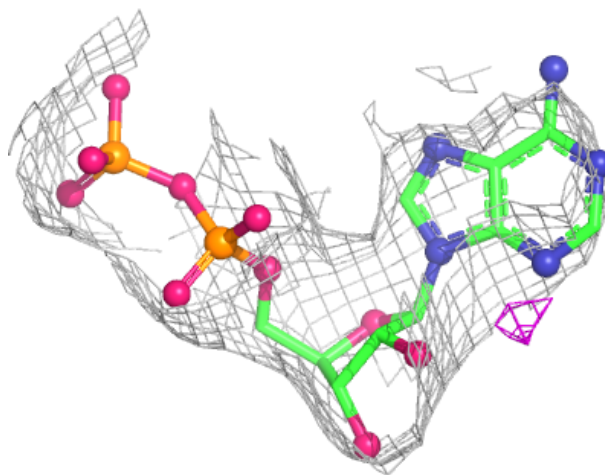
Electron density around ADP I 1450:

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



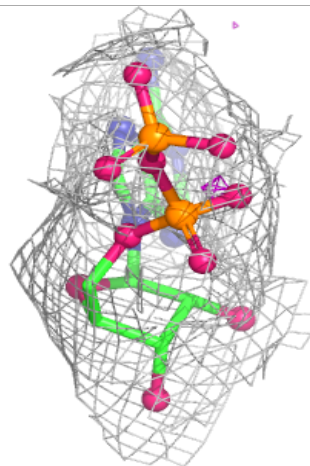
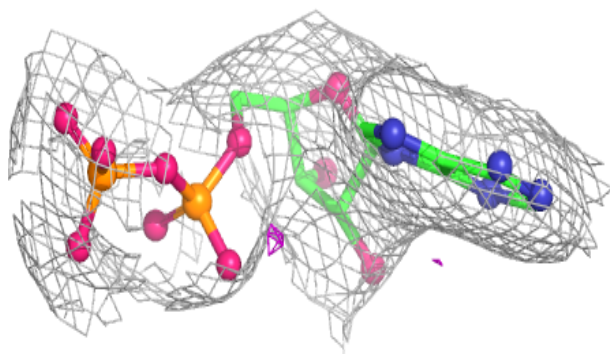
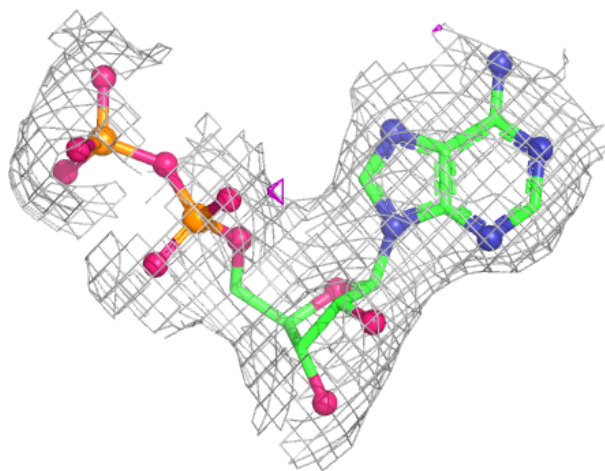
Electron density around ADP H 1450:

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



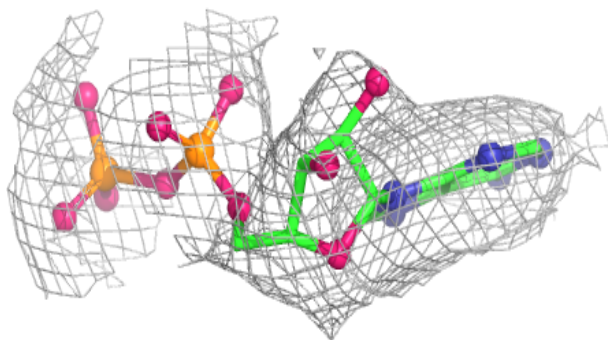
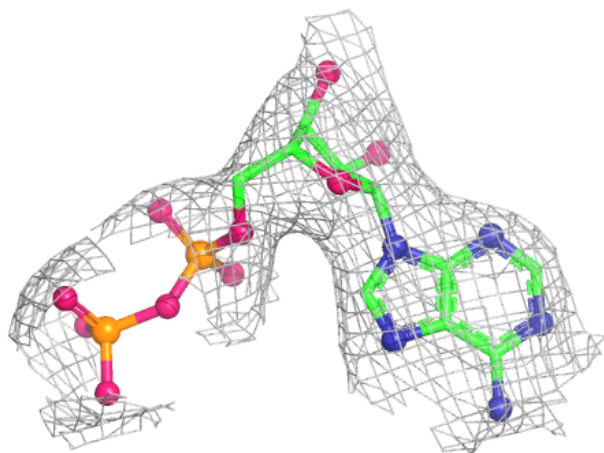
Electron density around ADP F 1450:

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



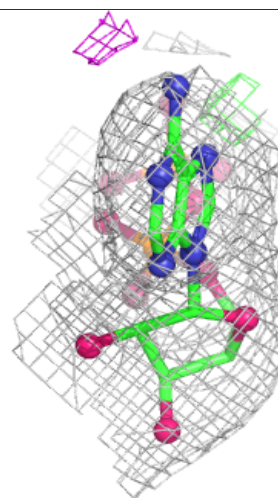
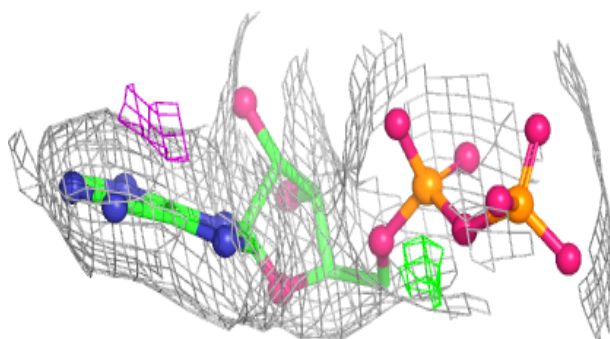
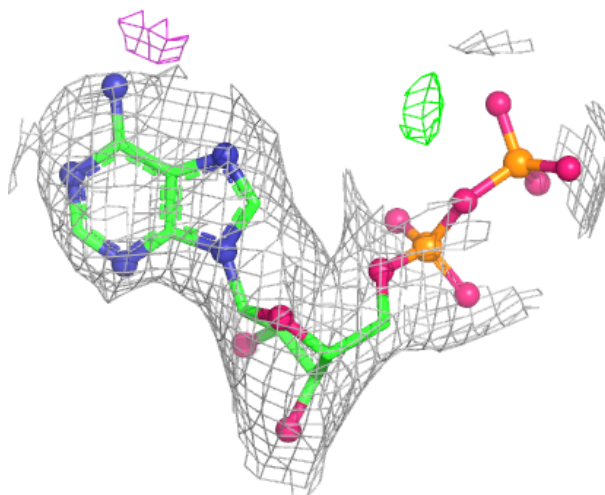
Electron density around ADP C 1450:

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



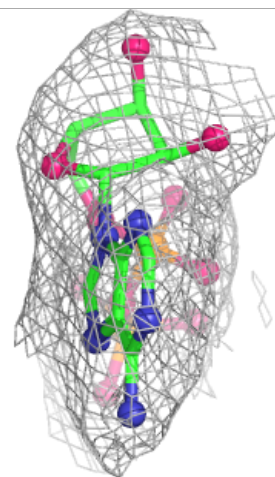
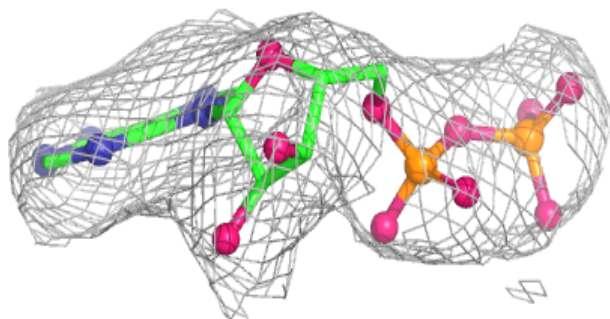
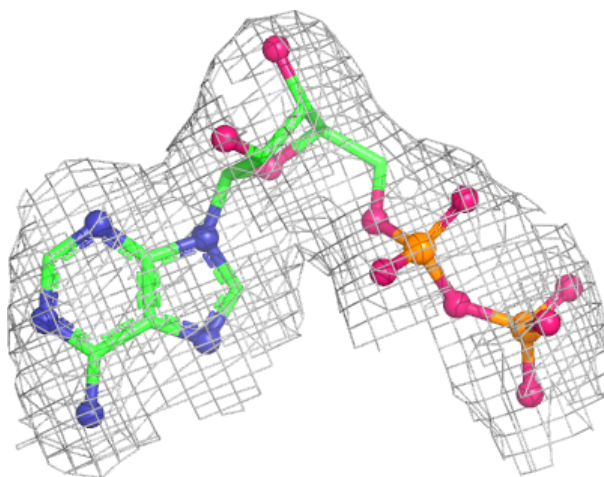
Electron density around ADP J 1450:

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



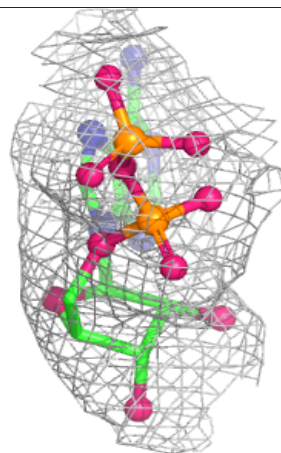
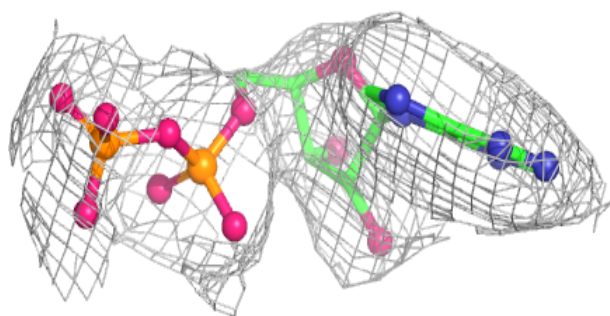
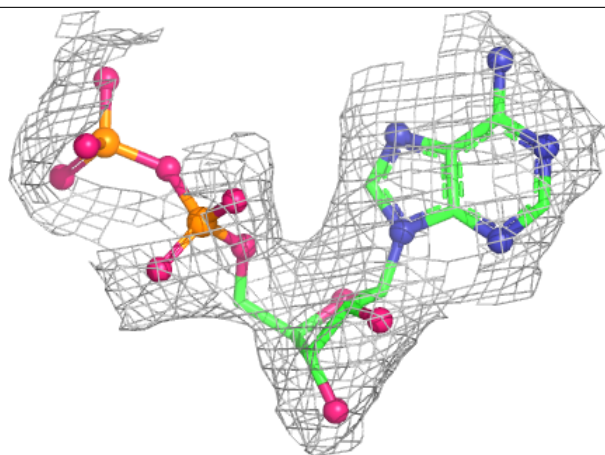
Electron density around ADP D 1450:

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



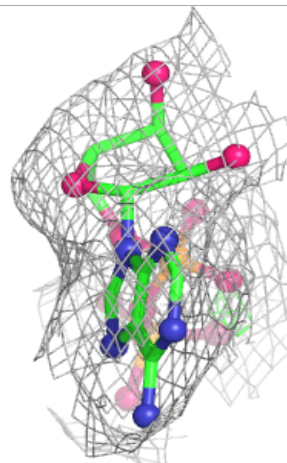
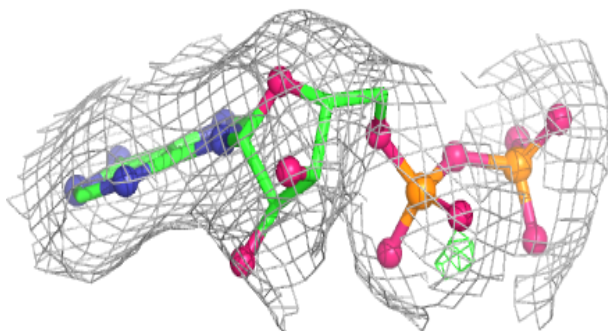
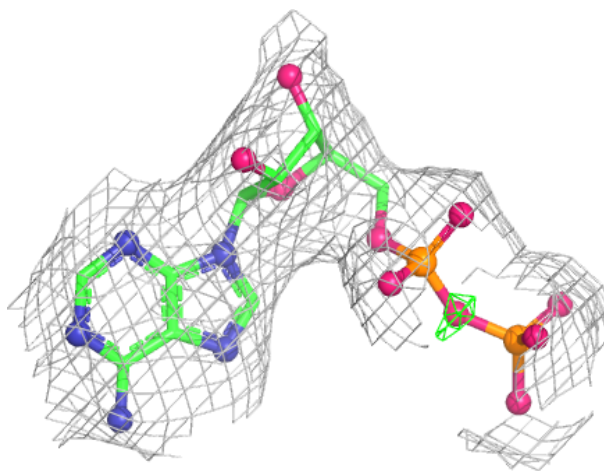
Electron density around ADP E 1450:

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



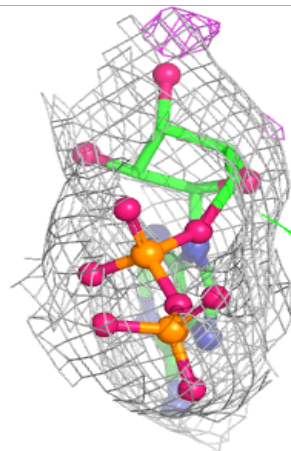
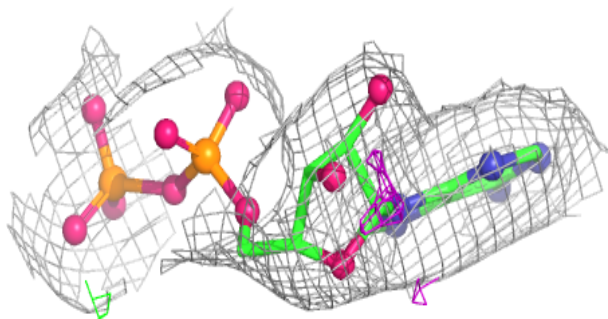
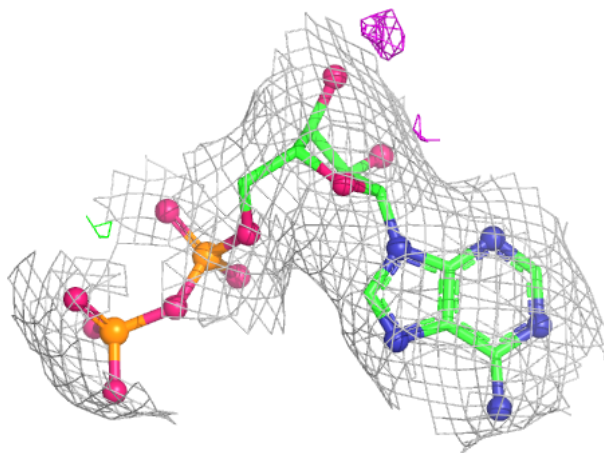
Electron density around ADP B 1450:

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



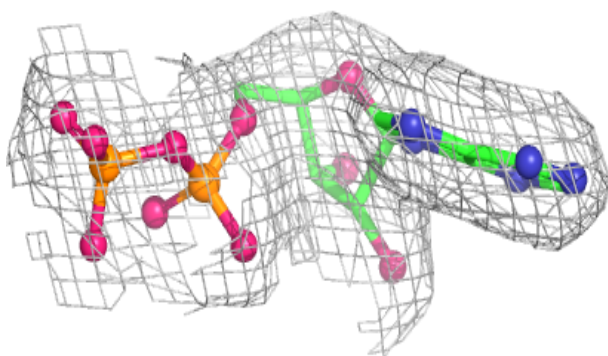
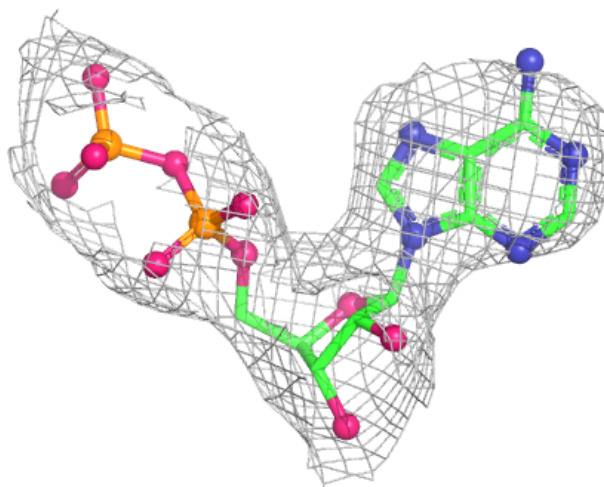
Electron density around ADP A 1450:

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



Electron density around ADP G 1450:

$2mF_o-DF_c$ (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.