



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 23, 2023 – 06:01 AM EDT

PDB ID : 3BLW
Title : Yeast Isocitrate Dehydrogenase with Citrate and AMP Bound in the Regulatory Subunits
Authors : Taylor, A.B.; Hu, G.; Hart, P.J.; McAlister-Henn, L.
Deposited on : 2007-12-11
Resolution : 4.30 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

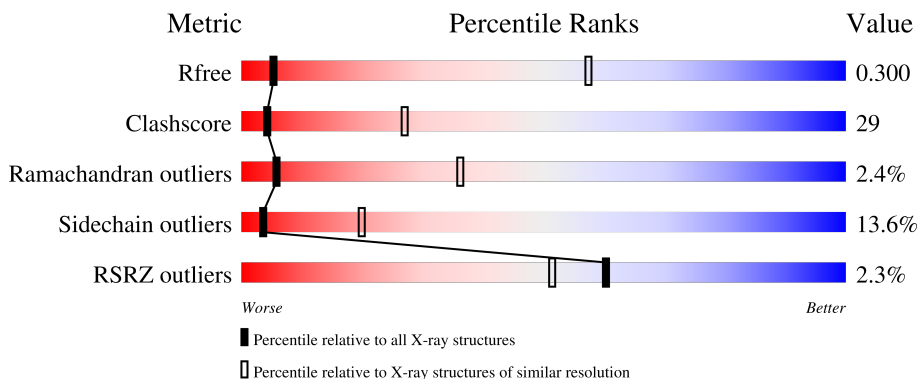
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1014 (4.80-3.80)
Clashscore	141614	1077 (4.80-3.80)
Ramachandran outliers	138981	1029 (4.80-3.80)
Sidechain outliers	138945	1012 (4.80-3.80)
RSRZ outliers	127900	1075 (4.90-3.70)

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	349	 54% 34% 6% • 6%
1	C	349	 56% 35% 6% • •
1	E	349	 54% 36% 6% • •
1	G	349	 54% 34% 6% • 6%
1	I	349	 53% 35% 5% • 6%

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Mol	Chain	Length	Quality of chain
1	K	349	
1	M	349	
1	O	349	
2	B	354	
2	D	354	
2	F	354	
2	H	354	
2	J	354	
2	L	354	
2	N	354	
2	P	354	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FLC	A	1001	-	-	X	-
3	FLC	C	1002	-	-	X	-
3	FLC	E	1003	-	-	X	-
3	FLC	G	1004	-	-	X	-
3	FLC	I	1005	-	-	X	-
3	FLC	K	1006	-	-	X	-
3	FLC	M	1007	-	-	X	-
3	FLC	O	1008	-	-	X	-
4	AMP	G	2004	-	-	-	X
4	AMP	K	2006	-	-	X	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 41694 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 Isocitrate dehydrogenase [NAD] subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	329	Total 2523	C 1594	N 440	O 482	S 7	0	0	0
1	C	338	Total 2599	C 1643	N 454	O 495	S 7	0	0	0
1	E	338	Total 2599	C 1643	N 454	O 495	S 7	0	0	0
1	G	329	Total 2523	C 1594	N 440	O 482	S 7	0	0	0
1	I	329	Total 2523	C 1594	N 440	O 482	S 7	0	0	0
1	K	337	Total 2590	C 1638	N 453	O 492	S 7	0	0	0
1	M	339	Total 2604	C 1646	N 455	O 496	S 7	0	0	0
1	O	330	Total 2527	C 1596	N 441	O 483	S 7	0	0	0

- Molecule 2 is a protein called Isocitrate dehydrogenase [NAD] subunit 2.

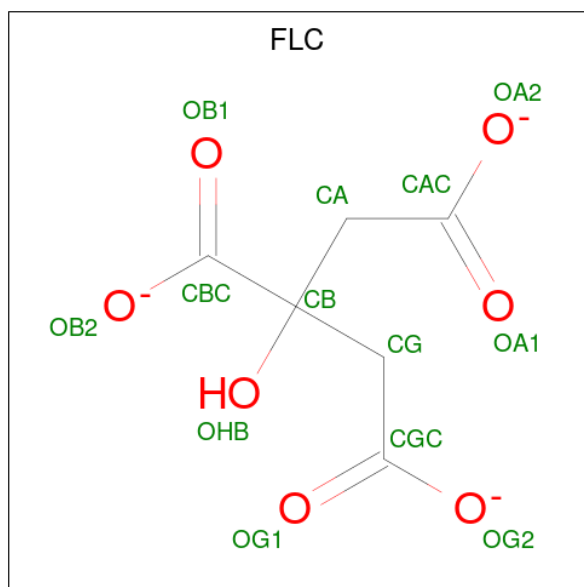
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	347	Total 2617	C 1652	N 449	O 510	S 6	0	0	0
2	D	347	Total 2617	C 1652	N 449	O 510	S 6	0	0	0
2	F	347	Total 2617	C 1652	N 449	O 510	S 6	0	0	0
2	H	346	Total 2608	C 1646	N 447	O 509	S 6	0	0	0
2	J	347	Total 2617	C 1652	N 449	O 510	S 6	0	0	0
2	L	346	Total 2608	C 1646	N 447	O 509	S 6	0	0	0

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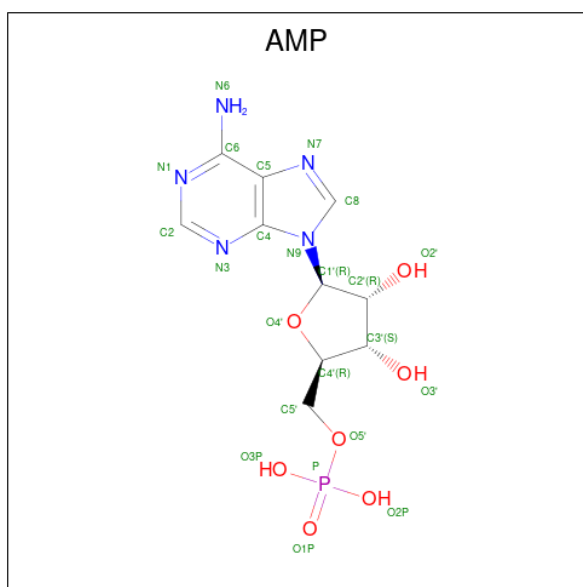
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	347	Total	C	N	O	S	0	0	0
			2617	1652	449	510	6			
2	P	347	Total	C	N	O	S	0	0	0
			2617	1652	449	510	6			

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7^-$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	C	1	Total	C	O	0	0
			13	6	7		
3	E	1	Total	C	O	0	0
			13	6	7		
3	G	1	Total	C	O	0	0
			13	6	7		
3	I	1	Total	C	O	0	0
			13	6	7		
3	K	1	Total	C	O	0	0
			13	6	7		
3	M	1	Total	C	O	0	0
			13	6	7		
3	O	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).

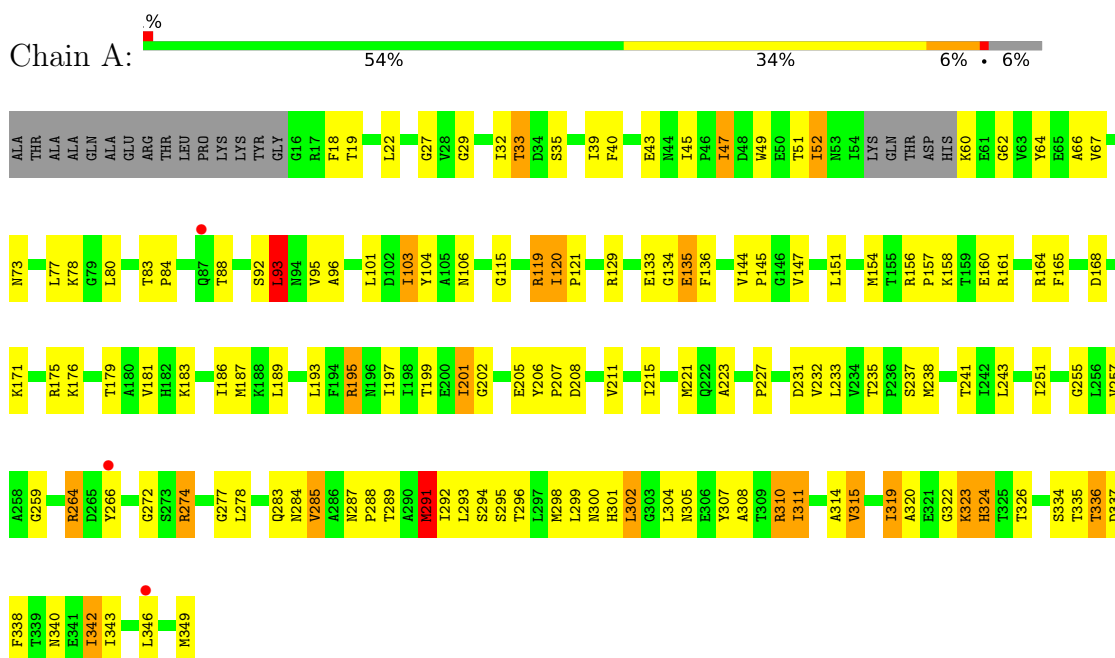


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	E	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	G	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	I	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	K	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	M	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	O	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

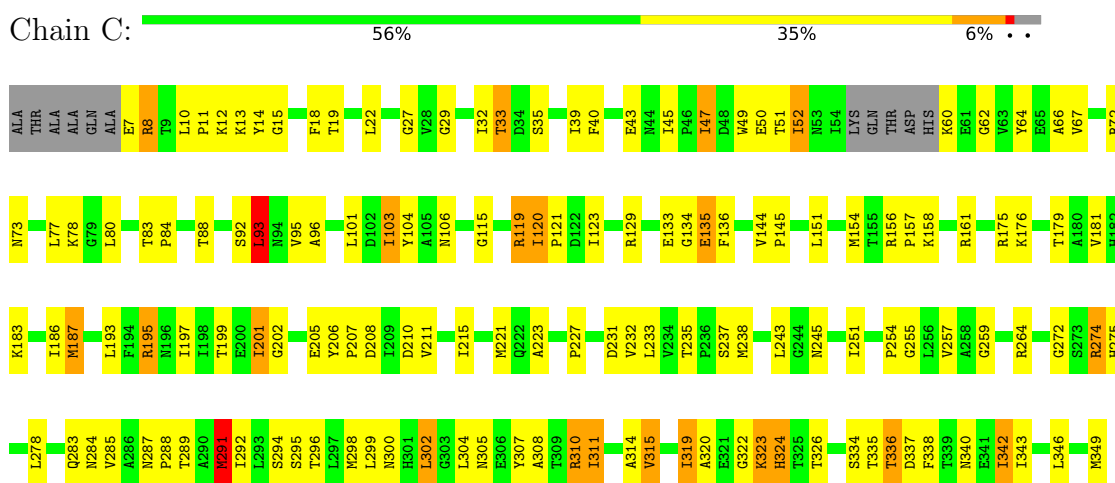
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

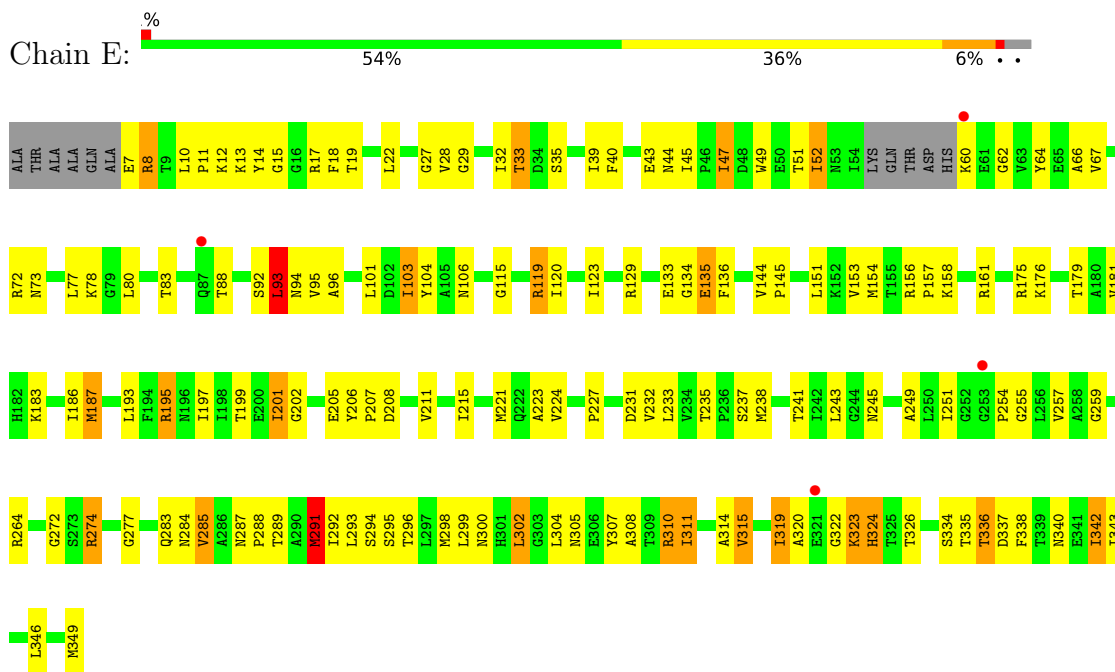
- Molecule 1: Isocitrate dehydrogenase [NAD] subunit 1



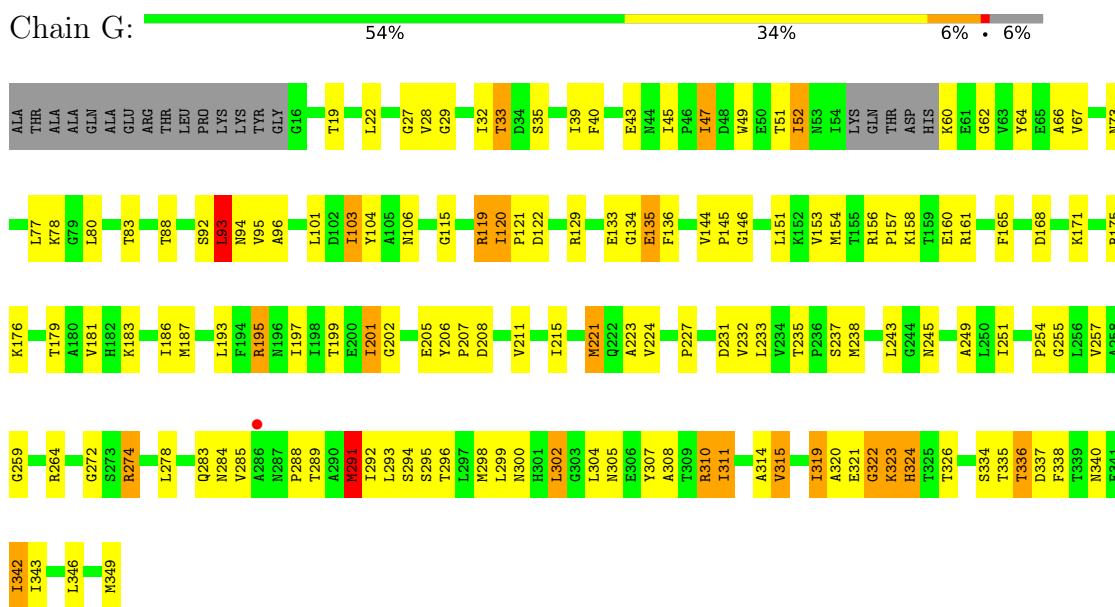
- Molecule 1: Isocitrate dehydrogenase [NAD] subunit 1



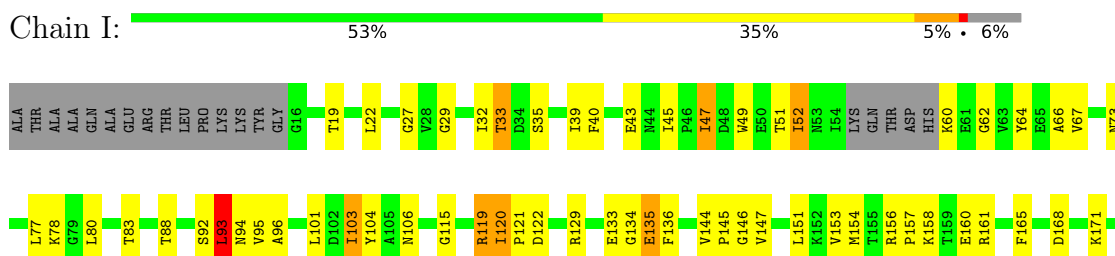
- Molecule 1: Isocitrate dehydrogenase [NAD] subunit 1

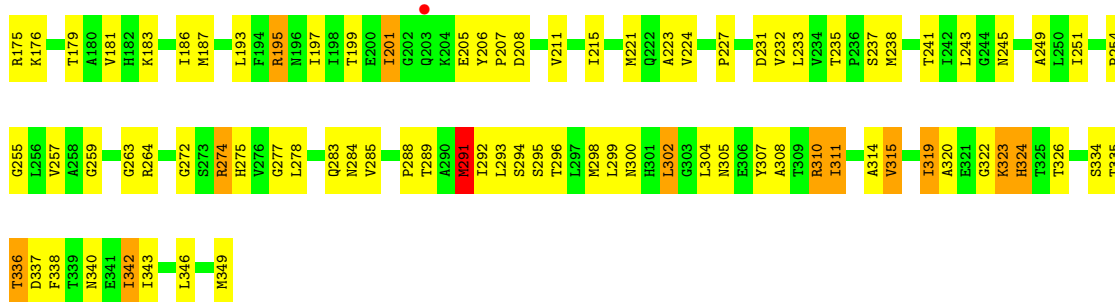


● Molecule 1: Isocitrate dehydrogenase [NAD] subunit 1

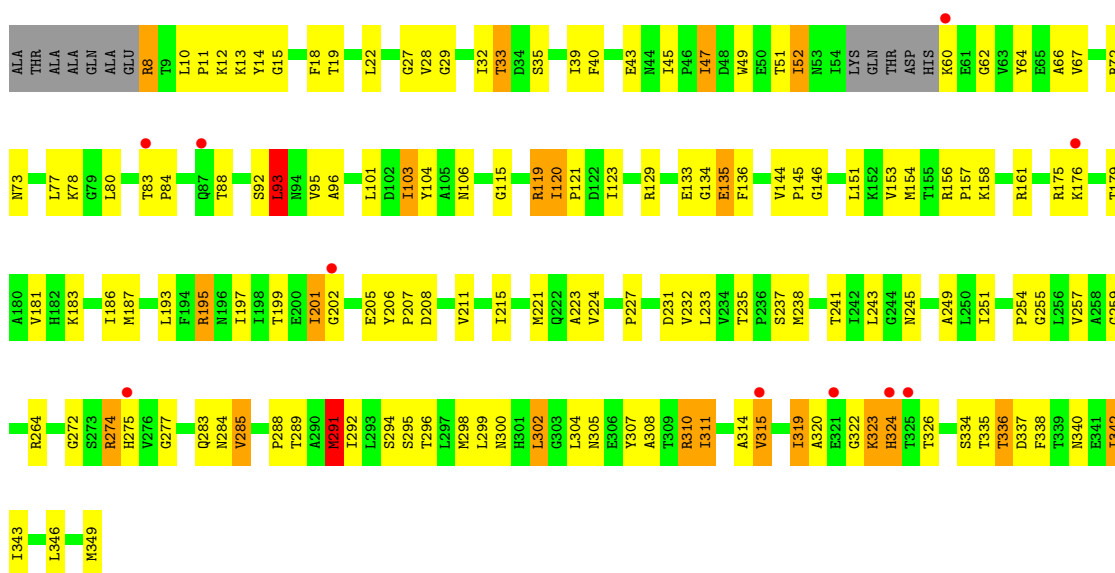


● Molecule 1: Isocitrate dehydrogenase [NAD] subunit 1

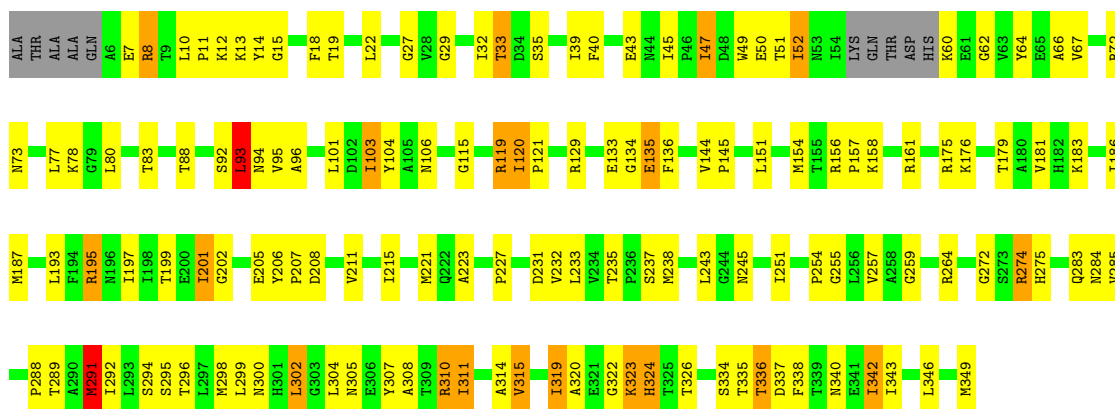




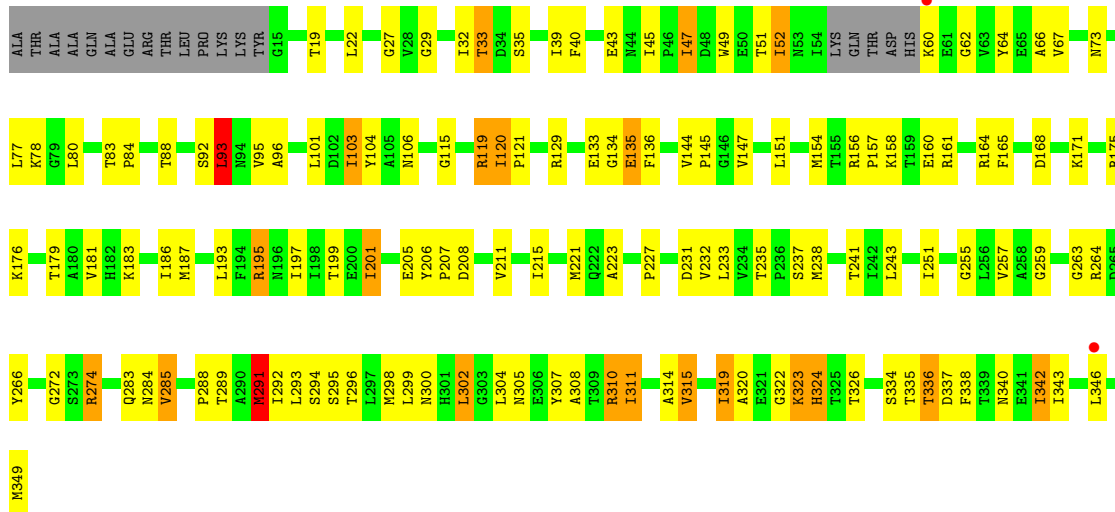
• Molecule 1: Isocitrate dehydrogenase [NAD] subunit 1



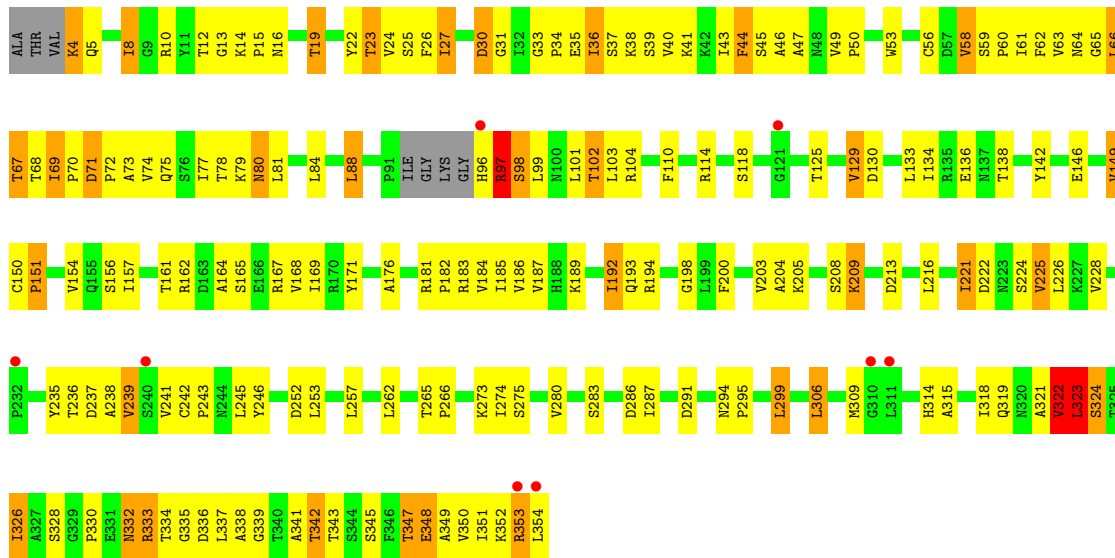
• Molecule 1: Isocitrate dehydrogenase [NAD] subunit 1



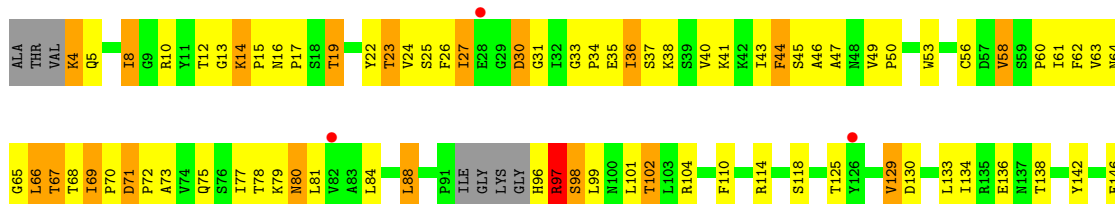
• Molecule 1: Isocitrate dehydrogenase [NAD] subunit 1

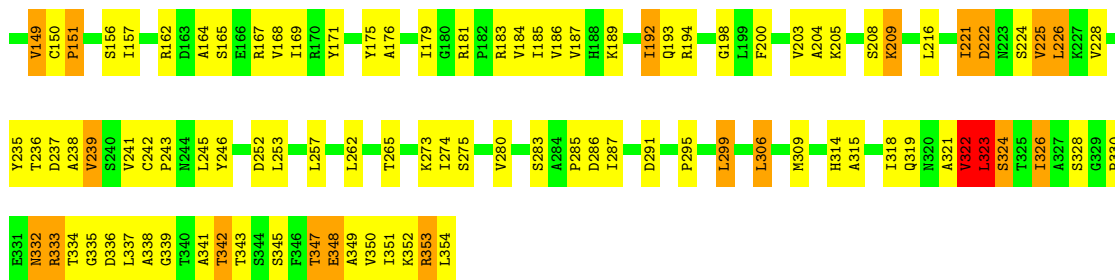


• Molecule 2: Isocitrate dehydrogenase [NAD] subunit 2

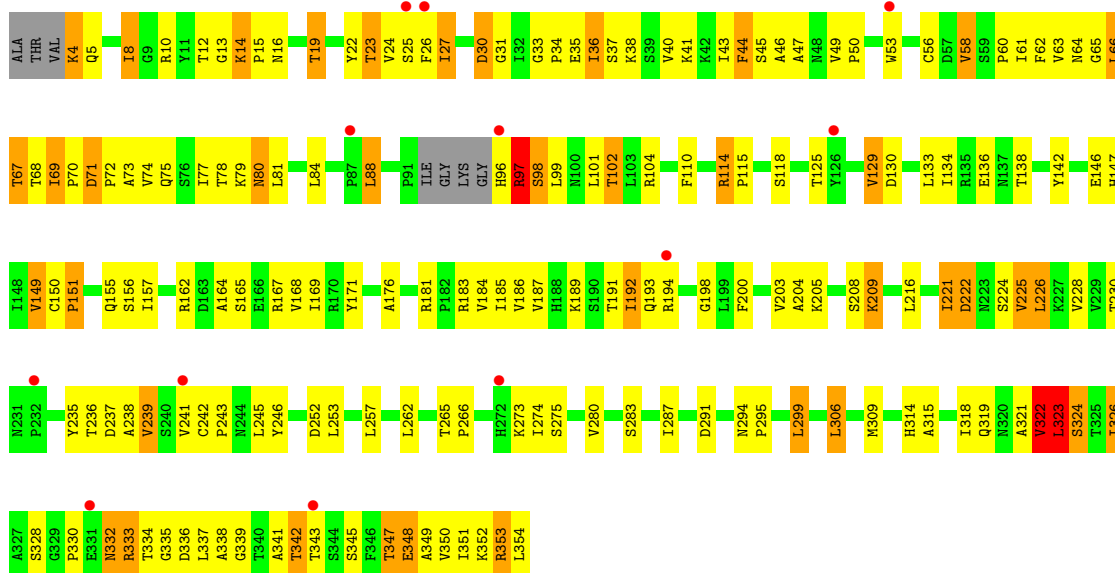


• Molecule 2: Isocitrate dehydrogenase [NAD] subunit 2

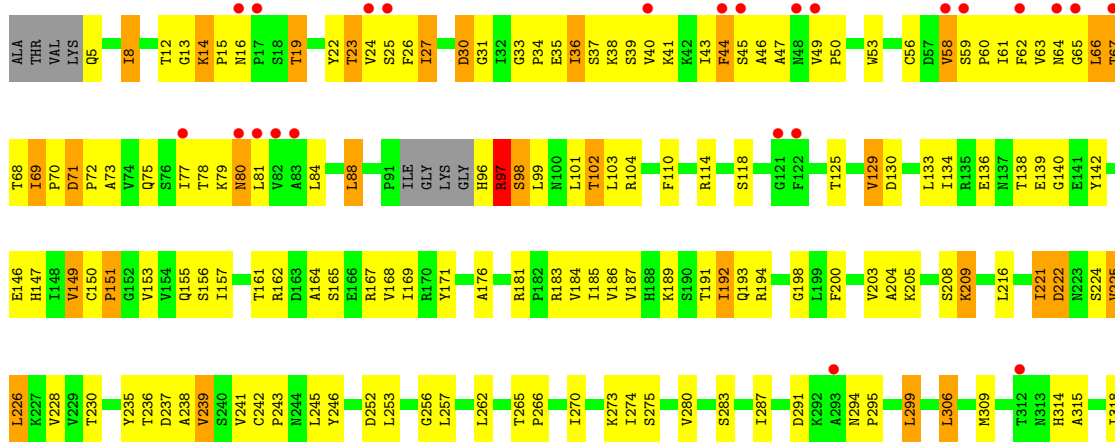




● Molecule 2: Isocitrate dehydrogenase [NAD] subunit 2

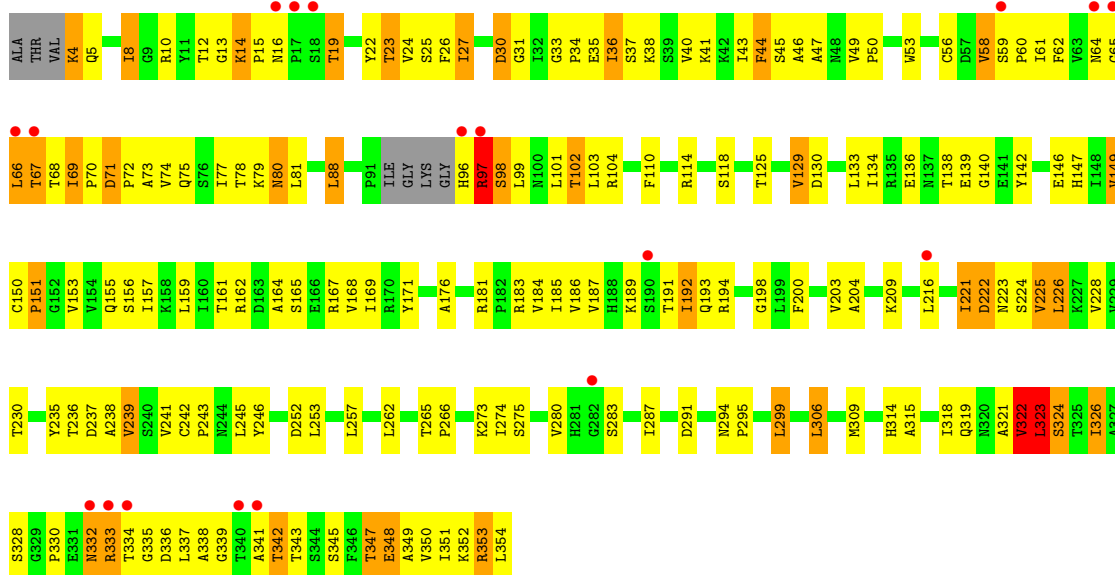


● Molecule 2: Isocitrate dehydrogenase [NAD] subunit 2

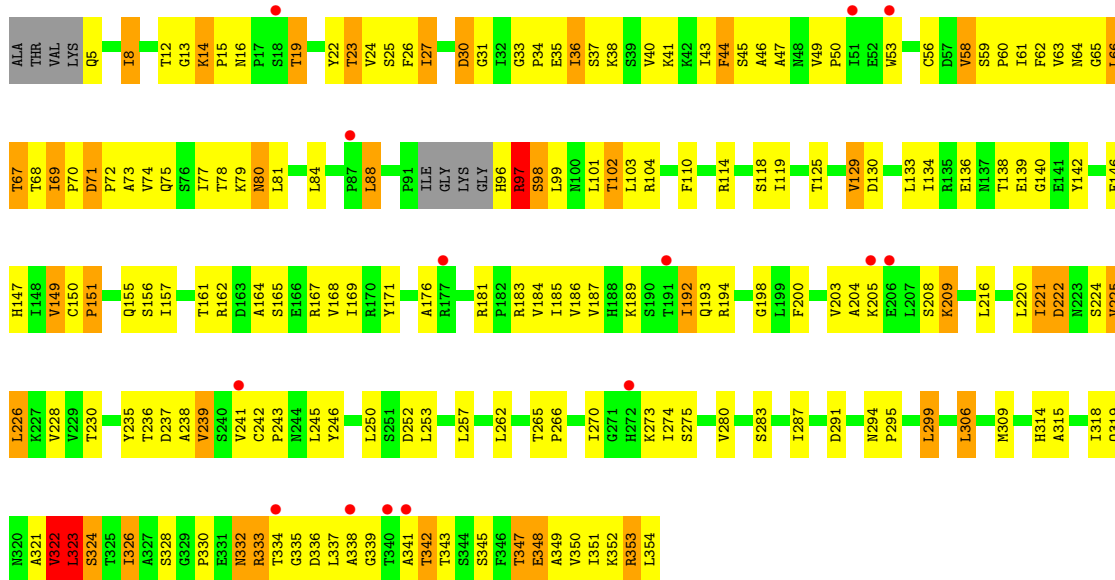




• Molecule 2: Isocitrate dehydrogenase [NAD] subunit 2

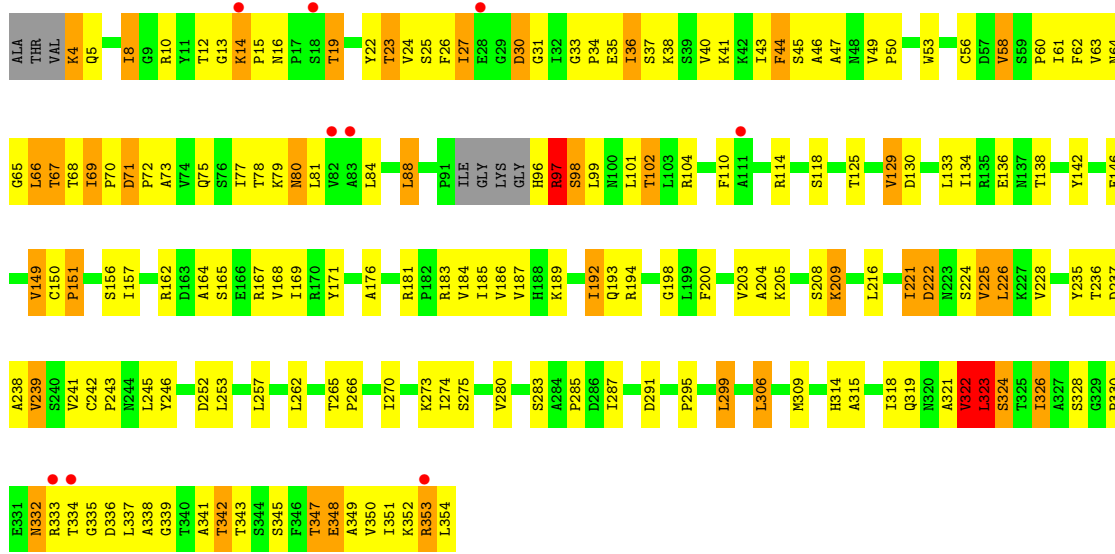


• Molecule 2: Isocitrate dehydrogenase [NAD] subunit 2

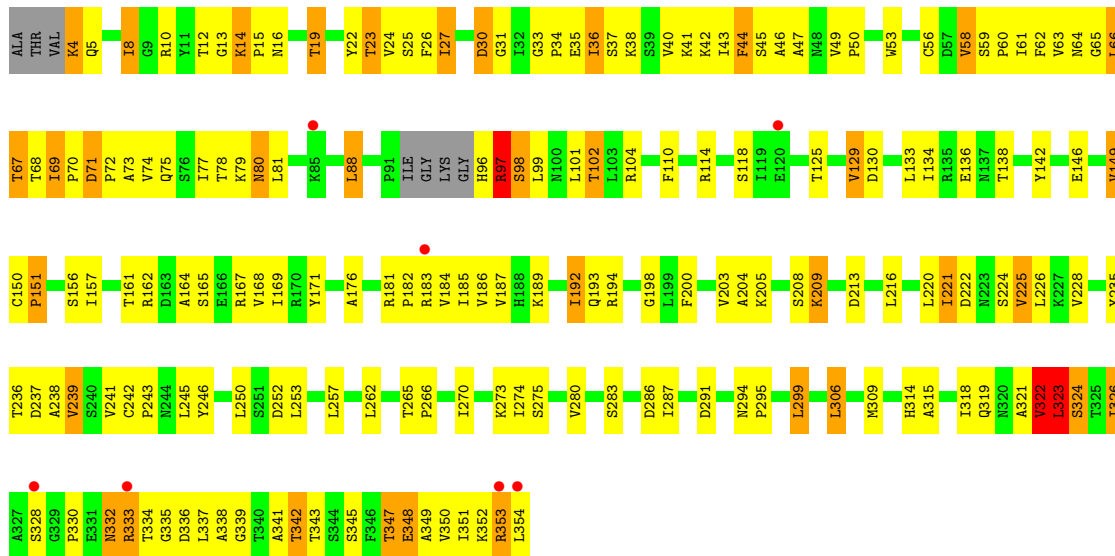


• Molecule 2: Isocitrate dehydrogenase [NAD] subunit 2





• Molecule 2: Isocitrate dehydrogenase [NAD] subunit 2



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	113.16Å 116.35Å 163.62Å 98.96° 110.23° 106.63°	Depositor
Resolution (Å)	49.38 – 4.30 49.39 – 4.30	Depositor EDS
% Data completeness (in resolution range)	90.7 (49.38-4.30) 90.8 (49.39-4.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 4.29Å)	Xtrriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.274 , 0.311 0.261 , 0.300	Depositor DCC
R_{free} test set	2238 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	139.2	Xtrriage
Anisotropy	0.281	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 124.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.000 for k,h,-h-k-l	Xtrriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	41694	wwPDB-VP
Average B, all atoms (Å ²)	190.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.65% 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: FLC, AMP

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	0.49	6/2565 (0.2%)	0.59	1/3467 (0.0%)
1	C	0.49	6/2643 (0.2%)	0.62	3/3571 (0.1%)
1	E	0.49	6/2643 (0.2%)	0.60	1/3571 (0.0%)
1	G	0.49	6/2565 (0.2%)	0.61	3/3467 (0.1%)
1	I	0.49	6/2565 (0.2%)	0.61	3/3467 (0.1%)
1	K	0.49	6/2634 (0.2%)	0.62	3/3559 (0.1%)
1	M	0.49	6/2648 (0.2%)	0.62	3/3578 (0.1%)
1	O	0.49	6/2569 (0.2%)	0.59	1/3472 (0.0%)
2	B	0.41	0/2663	0.57	0/3621
2	D	0.40	0/2663	0.57	0/3621
2	F	0.40	0/2663	0.57	0/3621
2	H	0.40	0/2654	0.57	0/3610
2	J	0.40	0/2663	0.57	0/3621
2	L	0.40	0/2654	0.57	0/3610
2	N	0.40	0/2663	0.57	0/3621
2	P	0.40	0/2663	0.57	0/3621
All	All	0.45	48/42118 (0.1%)	0.59	18/57098 (0.0%)

The worst 5 of 48 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	349	MET	CG-SD	5.84	1.96	1.81
1	E	349	MET	CG-SD	5.81	1.96	1.81
1	C	349	MET	CG-SD	5.80	1.96	1.81
1	K	349	MET	CG-SD	5.79	1.96	1.81
1	O	349	MET	CG-SD	5.78	1.96	1.81

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	264	ARG	NE-CZ-NH2	-5.95	117.32	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	264	ARG	NE-CZ-NH2	-5.95	117.32	120.30
1	I	264	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	K	264	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	G	264	ARG	NE-CZ-NH2	-5.91	117.34	120.30

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	2523	0	2559	151	0
1	C	2599	0	2641	142	0
1	E	2599	0	2641	158	0
1	G	2523	0	2559	134	1
1	I	2523	0	2559	141	0
1	K	2590	0	2635	155	0
1	M	2604	0	2646	142	0
1	O	2527	0	2562	133	0
2	B	2617	0	2662	180	2
2	D	2617	0	2662	193	0
2	F	2617	0	2662	186	0
2	H	2608	0	2649	185	0
2	J	2617	0	2662	192	0
2	L	2608	0	2649	194	0
2	N	2617	0	2662	171	2
2	P	2617	0	2662	200	1
3	A	13	0	5	5	0
3	C	13	0	5	4	0
3	E	13	0	5	4	0
3	G	13	0	5	5	0
3	I	13	0	5	5	0
3	K	13	0	5	4	0
3	M	13	0	5	6	0
3	O	13	0	5	5	0
4	A	23	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	23	0	12	2	0
4	E	23	0	12	6	0
4	G	23	0	12	1	0
4	I	23	0	12	3	0
4	K	23	0	12	9	0
4	M	23	0	12	3	0
4	O	23	0	12	0	0
All	All	41694	0	42208	2462	3

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 29.

The worst 5 of 2462 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:LYS:HZ2	1:E:72:ARG:NH2	1.27	1.32
2:B:213:ASP:HB3	1:I:122:ASP:OD2	1.23	1.27
2:D:285:PRO:HG3	2:P:286:ASP:OD2	1.42	1.20
2:D:285:PRO:CB	2:P:286:ASP:OD2	1.89	1.19
2:D:285:PRO:CG	2:P:286:ASP:OD2	1.91	1.19

All (3) 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)
2:B:286:ASP:OD2	2:N:285:PRO:CG[1_565]	1.88	0.32
2:B:286:ASP:OD2	2:N:285:PRO:CB[1_565]	1.90	0.30
1:G:122:ASP:OD2	2:P:213:ASP:CB[1_565]	2.15	0.05

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	325/349 (93%)	295 (91%)	27 (8%)	3 (1%)	17	56
1	C	334/349 (96%)	300 (90%)	31 (9%)	3 (1%)	17	56
1	E	334/349 (96%)	300 (90%)	31 (9%)	3 (1%)	17	56
1	G	325/349 (93%)	295 (91%)	27 (8%)	3 (1%)	17	56
1	I	325/349 (93%)	295 (91%)	27 (8%)	3 (1%)	17	56
1	K	333/349 (95%)	300 (90%)	30 (9%)	3 (1%)	17	56
1	M	335/349 (96%)	301 (90%)	31 (9%)	3 (1%)	17	56
1	O	326/349 (93%)	296 (91%)	27 (8%)	3 (1%)	17	56
2	B	343/354 (97%)	289 (84%)	42 (12%)	12 (4%)	3	29
2	D	343/354 (97%)	289 (84%)	41 (12%)	13 (4%)	3	27
2	F	343/354 (97%)	289 (84%)	41 (12%)	13 (4%)	3	27
2	H	342/354 (97%)	288 (84%)	41 (12%)	13 (4%)	3	27
2	J	343/354 (97%)	289 (84%)	41 (12%)	13 (4%)	3	27
2	L	342/354 (97%)	288 (84%)	41 (12%)	13 (4%)	3	27
2	N	343/354 (97%)	290 (84%)	40 (12%)	13 (4%)	3	27
2	P	343/354 (97%)	289 (84%)	41 (12%)	13 (4%)	3	27
All	All	5379/5624 (96%)	4693 (87%)	559 (10%)	127 (2%)	6	36

5 of 127 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	304	LEU
2	B	97	ARG
2	B	151	PRO
2	B	322	VAL
2	B	323	LEU

5.3.2 Protein sidechains [i](#)

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	274/289 (95%)	245 (89%)	29 (11%)	6	27
1	C	282/289 (98%)	253 (90%)	29 (10%)	7	27
1	E	282/289 (98%)	251 (89%)	31 (11%)	6	25
1	G	274/289 (95%)	247 (90%)	27 (10%)	8	29
1	I	274/289 (95%)	247 (90%)	27 (10%)	8	29
1	K	281/289 (97%)	251 (89%)	30 (11%)	6	27
1	M	282/289 (98%)	254 (90%)	28 (10%)	8	29
1	O	274/289 (95%)	245 (89%)	29 (11%)	6	27
2	B	293/297 (99%)	244 (83%)	49 (17%)	2	14
2	D	293/297 (99%)	244 (83%)	49 (17%)	2	14
2	F	293/297 (99%)	244 (83%)	49 (17%)	2	14
2	H	292/297 (98%)	244 (84%)	48 (16%)	2	14
2	J	293/297 (99%)	244 (83%)	49 (17%)	2	14
2	L	292/297 (98%)	244 (84%)	48 (16%)	2	14
2	N	293/297 (99%)	245 (84%)	48 (16%)	2	14
2	P	293/297 (99%)	244 (83%)	49 (17%)	2	14
All	All	4565/4688 (97%)	3946 (86%)	619 (14%)	3	20

5 of 619 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	348	GLU
2	P	19	THR
1	M	120	ILE
2	L	347	THR
2	N	192	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	245	ASN
2	N	64	ASN
1	K	301	HIS
1	M	106	ASN
2	N	223	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 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
3	FLC	G	1004	-	12,12,12	3.52	7 (58%)	17,17,17	1.54	1 (5%)
4	AMP	K	2006	-	22,25,25	0.98	1 (4%)	25,38,38	1.45	3 (12%)
4	AMP	C	2002	-	22,25,25	0.98	1 (4%)	25,38,38	1.45	3 (12%)
3	FLC	O	1008	-	12,12,12	3.52	8 (66%)	17,17,17	1.54	1 (5%)
3	FLC	A	1001	-	12,12,12	3.51	8 (66%)	17,17,17	1.55	1 (5%)
3	FLC	I	1005	-	12,12,12	3.50	7 (58%)	17,17,17	1.52	1 (5%)
3	FLC	E	1003	-	12,12,12	3.51	8 (66%)	17,17,17	1.54	1 (5%)
4	AMP	E	2003	-	22,25,25	0.98	1 (4%)	25,38,38	1.45	3 (12%)
3	FLC	C	1002	-	12,12,12	3.52	7 (58%)	17,17,17	1.55	1 (5%)
3	FLC	M	1007	-	12,12,12	3.52	8 (66%)	17,17,17	1.54	1 (5%)
4	AMP	M	2007	-	22,25,25	0.98	1 (4%)	25,38,38	1.45	3 (12%)
4	AMP	G	2004	-	22,25,25	0.98	1 (4%)	25,38,38	1.45	3 (12%)
4	AMP	I	2005	-	22,25,25	0.98	1 (4%)	25,38,38	1.45	3 (12%)
3	FLC	K	1006	-	12,12,12	3.52	7 (58%)	17,17,17	1.54	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	AMP	A	2001	-	22,25,25	0.98	1 (4%)	25,38,38	1.46	3 (12%)
4	AMP	O	2008	-	22,25,25	0.98	1 (4%)	25,38,38	1.45	3 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FLC	G	1004	-	-	8/16/16/16	-
4	AMP	K	2006	-	-	2/6/26/26	0/3/3/3
4	AMP	C	2002	-	-	5/6/26/26	0/3/3/3
3	FLC	O	1008	-	-	8/16/16/16	-
3	FLC	A	1001	-	-	8/16/16/16	-
3	FLC	I	1005	-	-	8/16/16/16	-
3	FLC	E	1003	-	-	8/16/16/16	-
4	AMP	E	2003	-	-	4/6/26/26	0/3/3/3
3	FLC	C	1002	-	-	8/16/16/16	-
3	FLC	M	1007	-	-	8/16/16/16	-
4	AMP	M	2007	-	-	4/6/26/26	0/3/3/3
4	AMP	G	2004	-	-	4/6/26/26	0/3/3/3
4	AMP	I	2005	-	-	1/6/26/26	0/3/3/3
3	FLC	K	1006	-	-	8/16/16/16	-
4	AMP	A	2001	-	-	1/6/26/26	0/3/3/3
4	AMP	O	2008	-	-	2/6/26/26	0/3/3/3

The worst 5 of 68 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1002	FLC	OB1-CBC	5.94	1.41	1.22
3	G	1004	FLC	OB1-CBC	5.90	1.41	1.22
3	E	1003	FLC	OB1-CBC	5.89	1.41	1.22
3	A	1001	FLC	OB1-CBC	5.89	1.41	1.22
3	O	1008	FLC	OG1-CGC	5.88	1.41	1.22

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	FLC	OB2-CBC-CB	4.12	120.21	113.05
3	C	1002	FLC	OB2-CBC-CB	4.10	120.17	113.05
3	E	1003	FLC	OB2-CBC-CB	4.08	120.14	113.05
3	K	1006	FLC	OB2-CBC-CB	4.08	120.13	113.05
3	M	1007	FLC	OB2-CBC-CB	4.08	120.13	113.05

There are no chirality outliers.

5 of 87 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	FLC	CA-CB-CG-CGC
3	A	1001	FLC	CBC-CB-CG-CGC
3	A	1001	FLC	OHB-CB-CG-CGC
3	C	1002	FLC	CA-CB-CG-CGC
3	C	1002	FLC	CBC-CB-CG-CGC

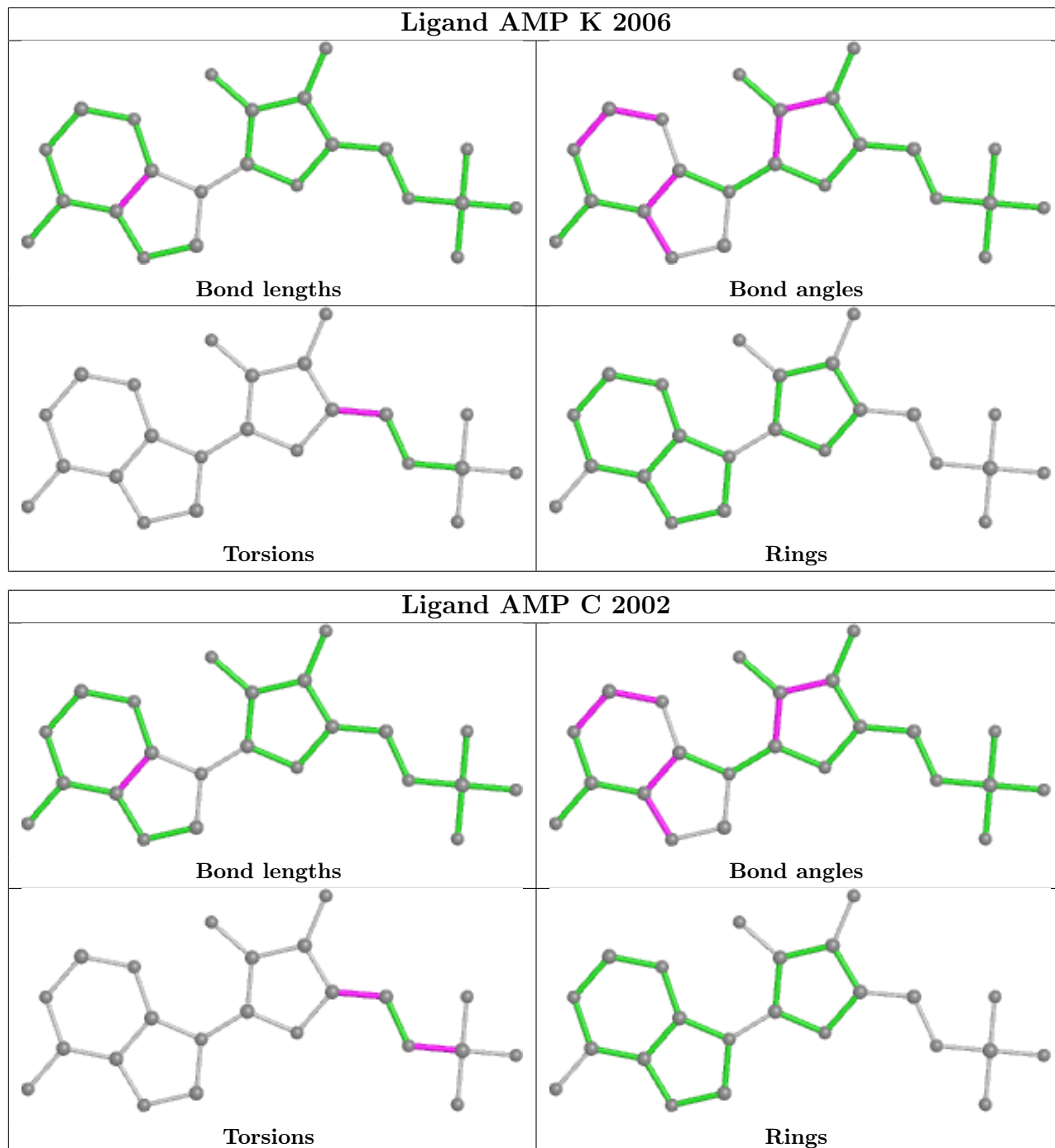
There are no ring outliers.

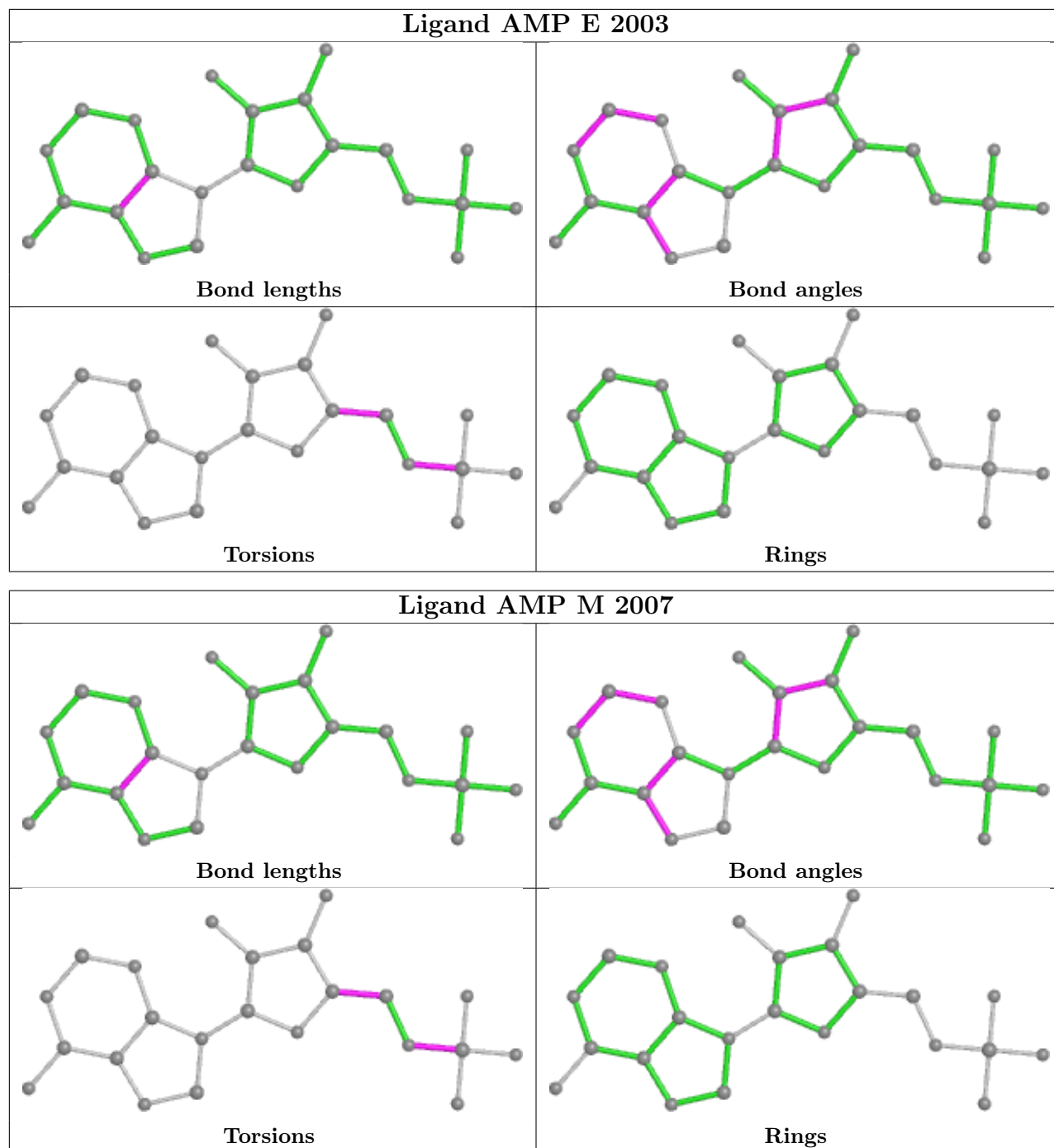
15 monomers are involved in 64 short contacts:

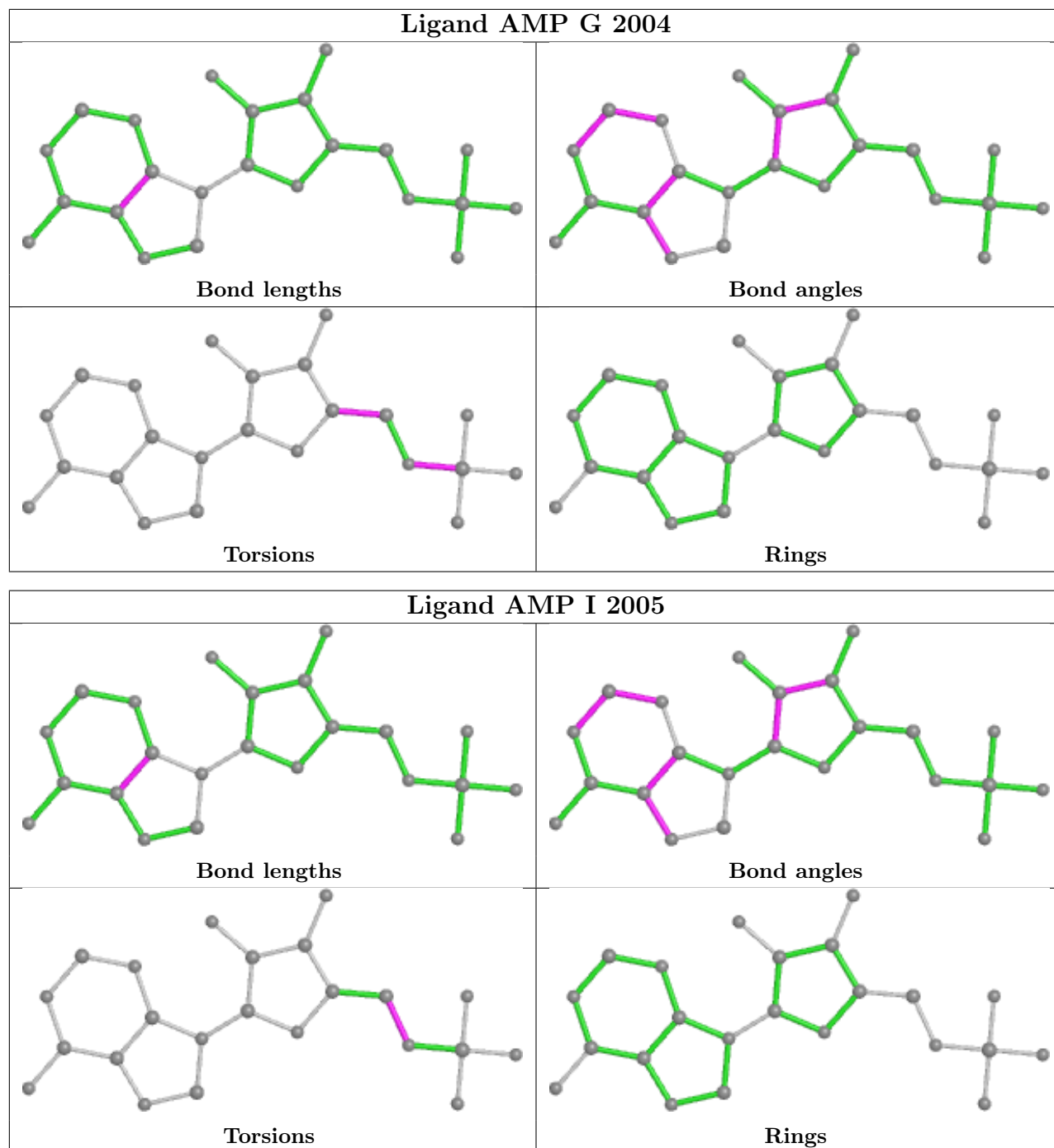
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1004	FLC	5	0
4	K	2006	AMP	9	0
4	C	2002	AMP	2	0
3	O	1008	FLC	5	0
3	A	1001	FLC	5	0
3	I	1005	FLC	5	0
3	E	1003	FLC	4	0
4	E	2003	AMP	6	0
3	C	1002	FLC	4	0
3	M	1007	FLC	6	0
4	M	2007	AMP	3	0
4	G	2004	AMP	1	0
4	I	2005	AMP	3	0
3	K	1006	FLC	4	0
4	A	2001	AMP	2	0

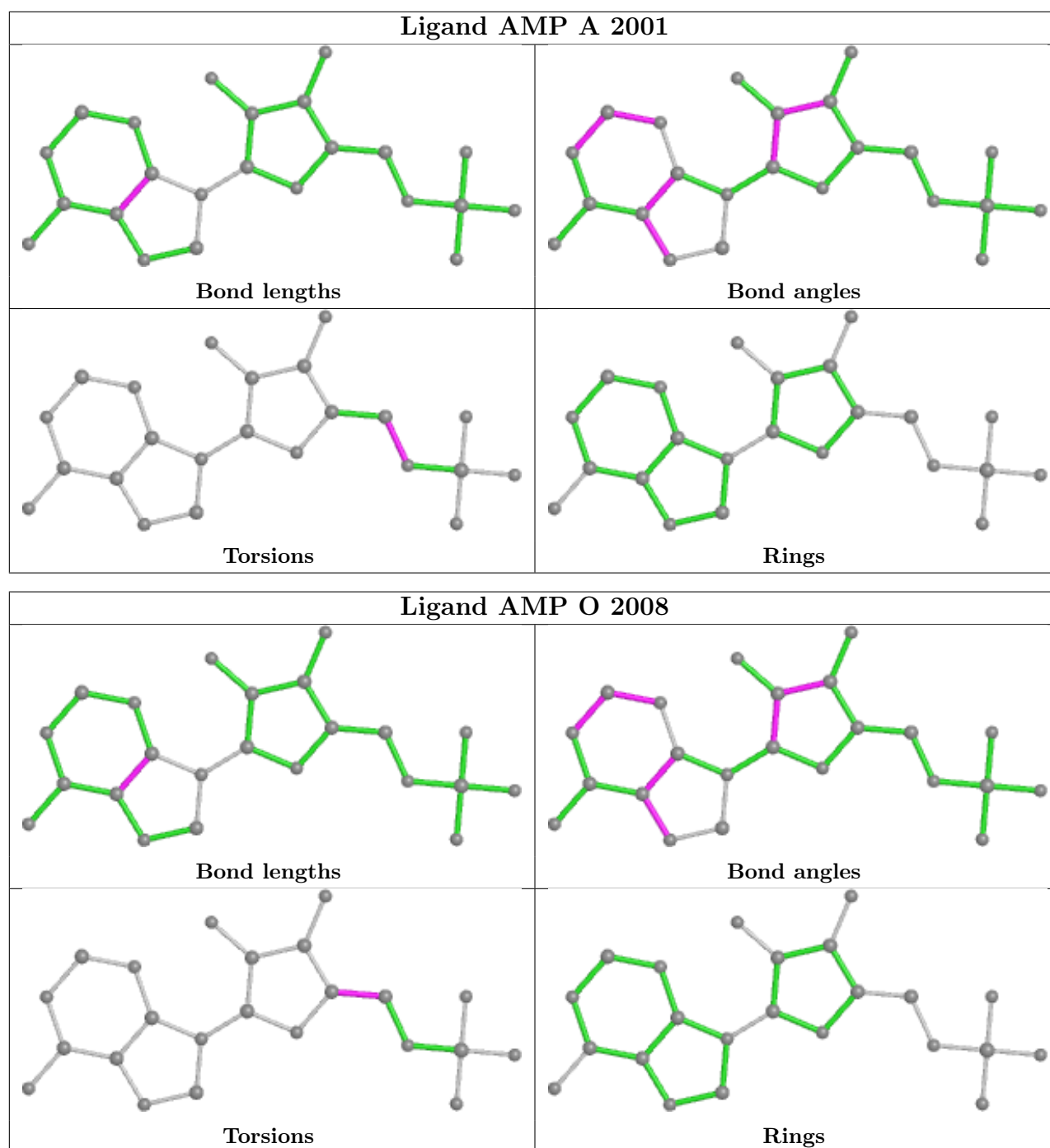
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	329/349 (94%)	-0.07	3 (0%) 84 77	120, 159, 225, 290	0
1	C	338/349 (96%)	-0.17	0 100 100	120, 151, 227, 309	0
1	E	338/349 (96%)	-0.03	4 (1%) 79 70	121, 194, 255, 288	0
1	G	329/349 (94%)	-0.16	1 (0%) 94 90	122, 185, 247, 313	0
1	I	329/349 (94%)	-0.18	1 (0%) 94 90	120, 176, 240, 331	0
1	K	337/349 (96%)	-0.01	10 (2%) 50 39	121, 195, 256, 286	0
1	M	339/349 (97%)	-0.14	0 100 100	120, 151, 210, 264	0
1	O	330/349 (94%)	-0.10	2 (0%) 89 84	120, 159, 234, 295	0
2	B	347/354 (98%)	-0.01	8 (2%) 60 51	120, 162, 233, 325	0
2	D	347/354 (98%)	-0.02	3 (0%) 84 77	121, 185, 269, 309	0
2	F	347/354 (98%)	0.15	12 (3%) 44 35	129, 234, 299, 325	0
2	H	346/354 (97%)	0.45	35 (10%) 7 7	123, 237, 317, 353	0
2	J	347/354 (98%)	0.31	18 (5%) 27 24	124, 229, 302, 357	0
2	L	346/354 (97%)	0.30	14 (4%) 38 30	137, 230, 289, 322	0
2	N	347/354 (98%)	0.10	9 (2%) 56 46	120, 186, 270, 304	0
2	P	347/354 (98%)	0.01	7 (2%) 65 56	120, 162, 234, 316	0
All	All	5443/5624 (96%)	0.03	127 (2%) 60 51	120, 185, 276, 357	0

The worst 5 of 127 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	82	VAL	6.4
2	J	65	GLY	4.7
2	N	28	GLU	4.5
2	H	59	SER	4.4
2	H	67	THR	4.3

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 monosaccharides in this entry.

6.4 Ligands [i](#)

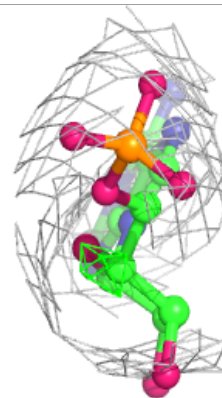
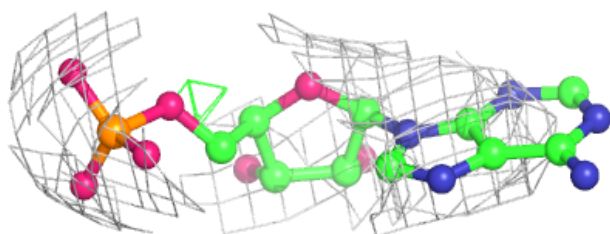
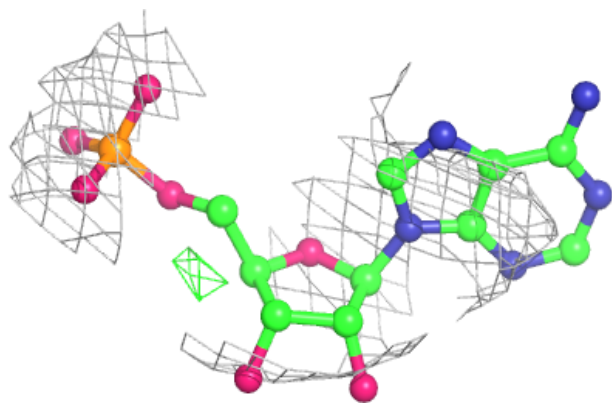
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	FLC	C	1002	13/13	0.71	0.34	179,179,179,179	0
4	AMP	K	2006	23/23	0.78	0.42	240,240,240,240	0
4	AMP	G	2004	23/23	0.79	0.49	164,164,164,164	0
4	AMP	E	2003	23/23	0.79	0.36	215,215,215,215	0
3	FLC	O	1008	13/13	0.81	0.34	148,148,148,148	0
3	FLC	I	1005	13/13	0.83	0.29	185,185,185,185	0
4	AMP	M	2007	23/23	0.83	0.29	137,137,137,137	0
3	FLC	A	1001	13/13	0.84	0.32	121,121,121,121	0
4	AMP	A	2001	23/23	0.84	0.26	150,150,150,150	0
4	AMP	I	2005	23/23	0.86	0.34	162,162,162,162	0
3	FLC	K	1006	13/13	0.86	0.32	155,155,155,155	0
3	FLC	M	1007	13/13	0.86	0.31	158,158,158,158	0
4	AMP	O	2008	23/23	0.87	0.26	135,135,135,135	0
3	FLC	G	1004	13/13	0.88	0.20	192,192,192,192	0
3	FLC	E	1003	13/13	0.88	0.31	173,173,173,173	0
4	AMP	C	2002	23/23	0.91	0.23	148,148,148,148	0

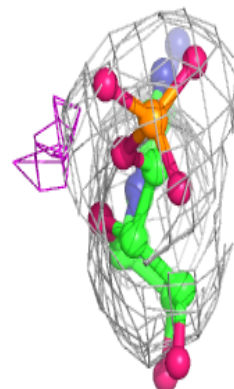
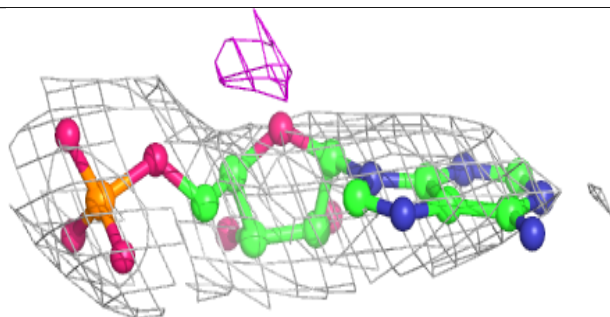
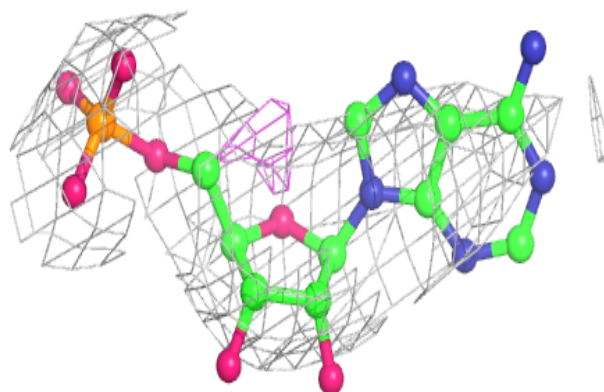
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AMP K 2006:

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

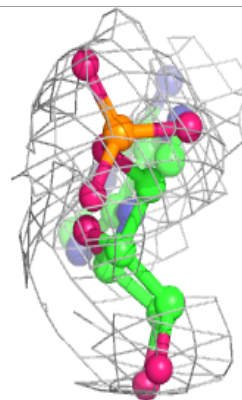
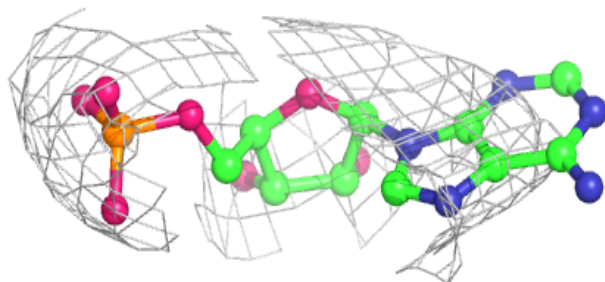
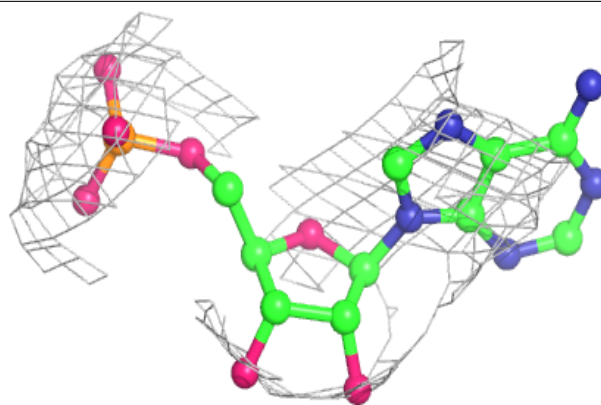
**Electron density around AMP G 2004:**

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

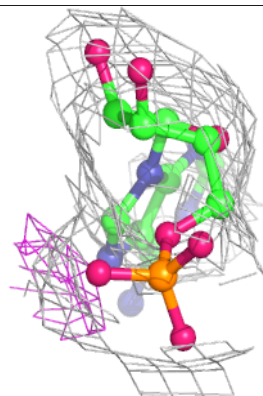
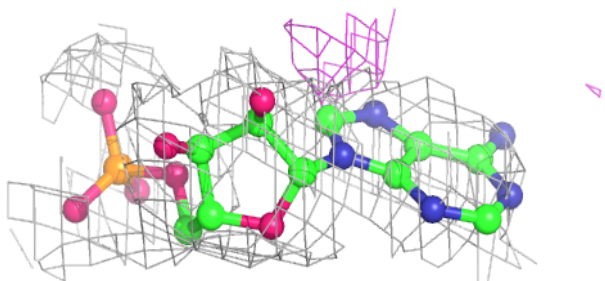
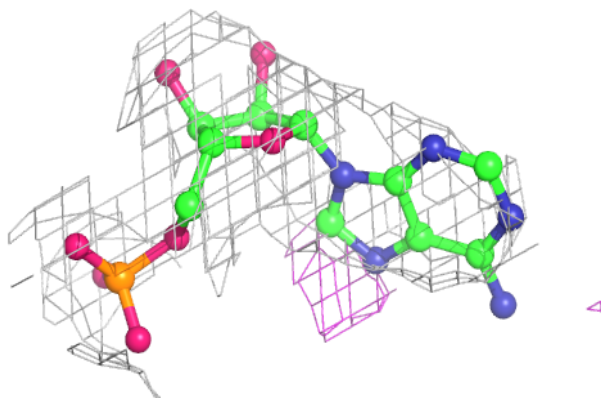


Electron density around AMP E 2003:

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

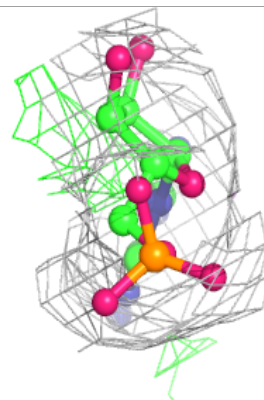
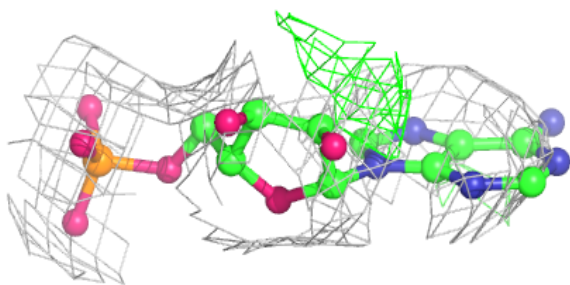
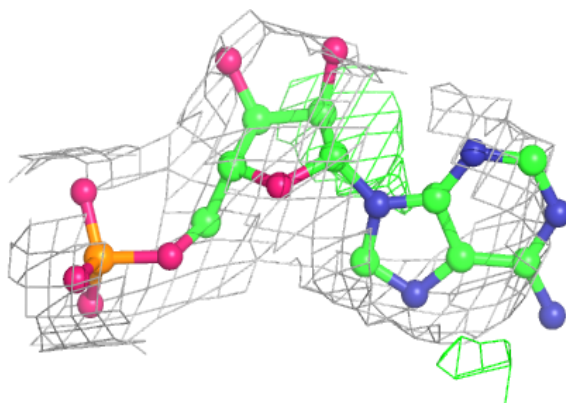
**Electron density around AMP M 2007:**

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

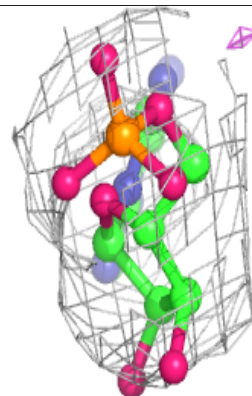
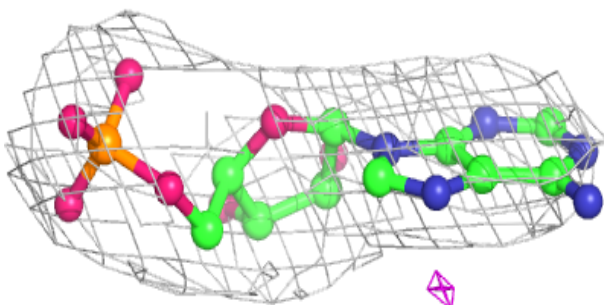
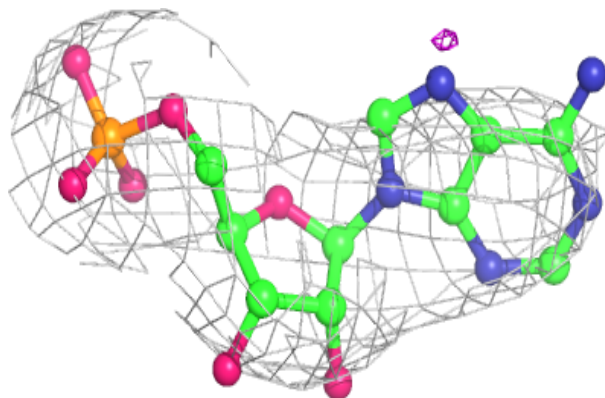


Electron density around AMP A 2001:

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

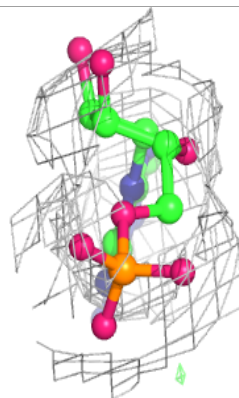
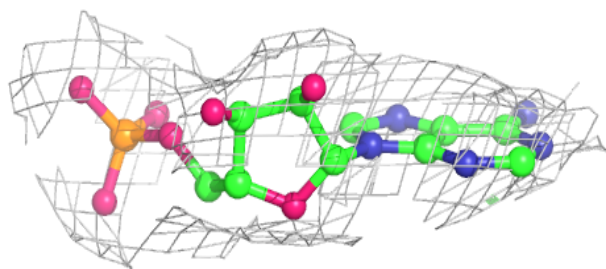
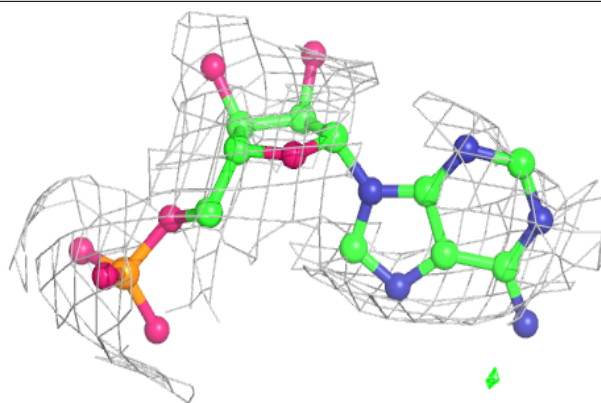
**Electron density around AMP I 2005:**

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

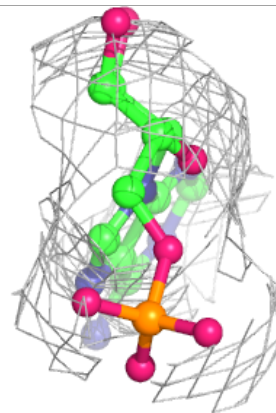
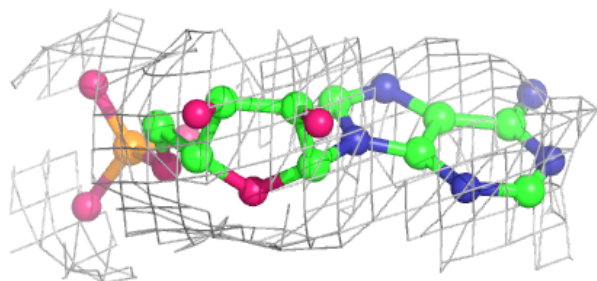
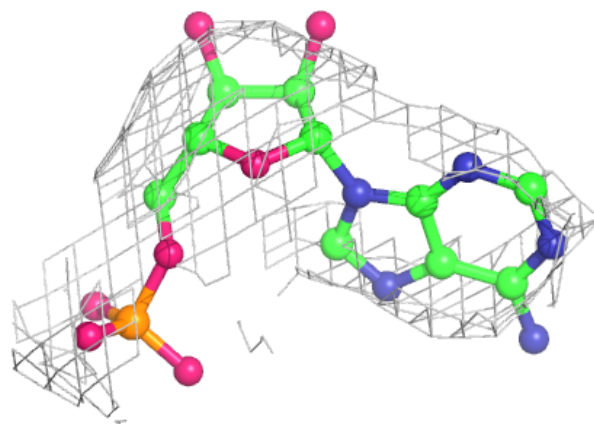


Electron density around AMP O 2008:

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

**Electron density around AMP C 2002:**

$2mF_o-DF_c$ (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.