



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 08:57 am GMT

PDB ID : 1GQ2
Title : MALIC ENZYME FROM PIGEON LIVER
Authors : Yang, Z.; Zhang, H.; Liang, T.
Deposited on : 2001-11-19
Resolution : 2.50 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

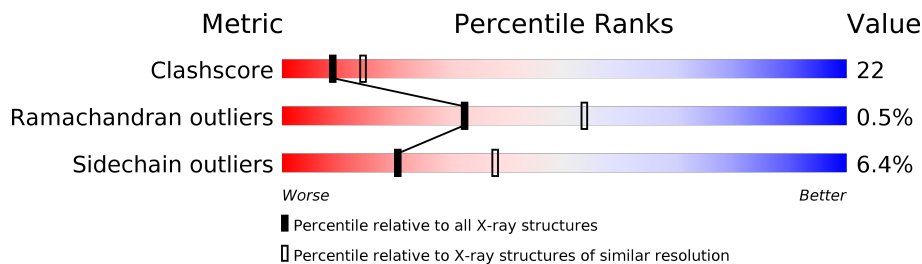
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)










The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	555	
1	B	555	
1	C	555	
1	D	555	
1	E	555	
1	F	555	
1	G	555	

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Mol	Chain	Length	Quality of chain
1	H	555	 62%35%.
1	I	555	 64%33%.
1	J	555	 64%33%.
1	K	555	 58%39%.
1	L	555	 58%38%.
1	M	555	 63%34%.
1	N	555	 60%36%.
1	O	555	 62%35%.
1	P	555	 64%32%.

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	OXL	C	1582	-	-	X	-
3	OXL	D	1582	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 71519 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 MALIC ENZYME.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	B	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	C	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	D	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	E	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	F	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	G	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	H	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	I	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	J	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	K	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	L	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	M	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	N	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	O	555	Total	C	N	O	S	Se	0	0	0
			4345	2772	742	806	11	14			
1	P	555	Total	C	N	O	S	Se	0	0	0
			4346	2772	742	807	11	14			

There are 224 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	MSE	MET	MODIFIED RESIDUE	UNP P40927
A	86	MSE	MET	MODIFIED RESIDUE	UNP P40927
A	108	MSE	MET	MODIFIED RESIDUE	UNP P40927
A	146	MSE	MET	MODIFIED RESIDUE	UNP P40927
A	177	MSE	MET	MODIFIED RESIDUE	UNP P40927
A	202	MSE	MET	MODIFIED RESIDUE	UNP P40927
A	239	MSE	MET	MODIFIED RESIDUE	UNP P40927
A	248	MSE	MET	MODIFIED RESIDUE	UNP P40927
A	325	MSE	MET	MODIFIED RESIDUE	UNP P40927
A	327	MSE	MET	MODIFIED RESIDUE	UNP P40927
A	343	MSE	MET	MODIFIED RESIDUE	UNP P40927
A	374	MSE	MET	MODIFIED RESIDUE	UNP P40927
A	407	MSE	MET	MODIFIED RESIDUE	UNP P40927
A	577	MSE	MET	MODIFIED RESIDUE	UNP P40927
B	38	MSE	MET	MODIFIED RESIDUE	UNP P40927
B	86	MSE	MET	MODIFIED RESIDUE	UNP P40927
B	108	MSE	MET	MODIFIED RESIDUE	UNP P40927
B	146	MSE	MET	MODIFIED RESIDUE	UNP P40927
B	177	MSE	MET	MODIFIED RESIDUE	UNP P40927
B	202	MSE	MET	MODIFIED RESIDUE	UNP P40927
B	239	MSE	MET	MODIFIED RESIDUE	UNP P40927
B	248	MSE	MET	MODIFIED RESIDUE	UNP P40927
B	325	MSE	MET	MODIFIED RESIDUE	UNP P40927
B	327	MSE	MET	MODIFIED RESIDUE	UNP P40927
B	343	MSE	MET	MODIFIED RESIDUE	UNP P40927
B	374	MSE	MET	MODIFIED RESIDUE	UNP P40927
B	407	MSE	MET	MODIFIED RESIDUE	UNP P40927
B	577	MSE	MET	MODIFIED RESIDUE	UNP P40927
C	38	MSE	MET	MODIFIED RESIDUE	UNP P40927
C	86	MSE	MET	MODIFIED RESIDUE	UNP P40927
C	108	MSE	MET	MODIFIED RESIDUE	UNP P40927
C	146	MSE	MET	MODIFIED RESIDUE	UNP P40927
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C	343	MSE	MET	MODIFIED RESIDUE	UNP P40927
C	374	MSE	MET	MODIFIED RESIDUE	UNP P40927
C	407	MSE	MET	MODIFIED RESIDUE	UNP P40927
C	577	MSE	MET	MODIFIED RESIDUE	UNP P40927

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Chain	Residue	Modelled	Actual	Comment	Reference
D	38	MSE	MET	MODIFIED RESIDUE	UNP P40927
D	86	MSE	MET	MODIFIED RESIDUE	UNP P40927
D	108	MSE	MET	MODIFIED RESIDUE	UNP P40927
D	146	MSE	MET	MODIFIED RESIDUE	UNP P40927
D	177	MSE	MET	MODIFIED RESIDUE	UNP P40927
D	202	MSE	MET	MODIFIED RESIDUE	UNP P40927
D	239	MSE	MET	MODIFIED RESIDUE	UNP P40927
D	248	MSE	MET	MODIFIED RESIDUE	UNP P40927
D	325	MSE	MET	MODIFIED RESIDUE	UNP P40927
D	327	MSE	MET	MODIFIED RESIDUE	UNP P40927
D	343	MSE	MET	MODIFIED RESIDUE	UNP P40927
D	374	MSE	MET	MODIFIED RESIDUE	UNP P40927
D	407	MSE	MET	MODIFIED RESIDUE	UNP P40927
D	577	MSE	MET	MODIFIED RESIDUE	UNP P40927
E	38	MSE	MET	MODIFIED RESIDUE	UNP P40927
E	86	MSE	MET	MODIFIED RESIDUE	UNP P40927
E	108	MSE	MET	MODIFIED RESIDUE	UNP P40927
E	146	MSE	MET	MODIFIED RESIDUE	UNP P40927
E	177	MSE	MET	MODIFIED RESIDUE	UNP P40927
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E	374	MSE	MET	MODIFIED RESIDUE	UNP P40927
E	407	MSE	MET	MODIFIED RESIDUE	UNP P40927
E	577	MSE	MET	MODIFIED RESIDUE	UNP P40927
F	38	MSE	MET	MODIFIED RESIDUE	UNP P40927
F	86	MSE	MET	MODIFIED RESIDUE	UNP P40927
F	108	MSE	MET	MODIFIED RESIDUE	UNP P40927
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F	327	MSE	MET	MODIFIED RESIDUE	UNP P40927
F	343	MSE	MET	MODIFIED RESIDUE	UNP P40927
F	374	MSE	MET	MODIFIED RESIDUE	UNP P40927
F	407	MSE	MET	MODIFIED RESIDUE	UNP P40927
F	577	MSE	MET	MODIFIED RESIDUE	UNP P40927

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Chain	Residue	Modelled	Actual	Comment	Reference
G	38	MSE	MET	MODIFIED RESIDUE	UNP P40927
G	86	MSE	MET	MODIFIED RESIDUE	UNP P40927
G	108	MSE	MET	MODIFIED RESIDUE	UNP P40927
G	146	MSE	MET	MODIFIED RESIDUE	UNP P40927
G	177	MSE	MET	MODIFIED RESIDUE	UNP P40927
G	202	MSE	MET	MODIFIED RESIDUE	UNP P40927
G	239	MSE	MET	MODIFIED RESIDUE	UNP P40927
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G	325	MSE	MET	MODIFIED RESIDUE	UNP P40927
G	327	MSE	MET	MODIFIED RESIDUE	UNP P40927
G	343	MSE	MET	MODIFIED RESIDUE	UNP P40927
G	374	MSE	MET	MODIFIED RESIDUE	UNP P40927
G	407	MSE	MET	MODIFIED RESIDUE	UNP P40927
G	577	MSE	MET	MODIFIED RESIDUE	UNP P40927
H	38	MSE	MET	MODIFIED RESIDUE	UNP P40927
H	86	MSE	MET	MODIFIED RESIDUE	UNP P40927
H	108	MSE	MET	MODIFIED RESIDUE	UNP P40927
H	146	MSE	MET	MODIFIED RESIDUE	UNP P40927
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H	407	MSE	MET	MODIFIED RESIDUE	UNP P40927
H	577	MSE	MET	MODIFIED RESIDUE	UNP P40927
I	38	MSE	MET	MODIFIED RESIDUE	UNP P40927
I	86	MSE	MET	MODIFIED RESIDUE	UNP P40927
I	108	MSE	MET	MODIFIED RESIDUE	UNP P40927
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I	327	MSE	MET	MODIFIED RESIDUE	UNP P40927
I	343	MSE	MET	MODIFIED RESIDUE	UNP P40927
I	374	MSE	MET	MODIFIED RESIDUE	UNP P40927
I	407	MSE	MET	MODIFIED RESIDUE	UNP P40927
I	577	MSE	MET	MODIFIED RESIDUE	UNP P40927

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Chain	Residue	Modelled	Actual	Comment	Reference
J	38	MSE	MET	MODIFIED RESIDUE	UNP P40927
J	86	MSE	MET	MODIFIED RESIDUE	UNP P40927
J	108	MSE	MET	MODIFIED RESIDUE	UNP P40927
J	146	MSE	MET	MODIFIED RESIDUE	UNP P40927
J	177	MSE	MET	MODIFIED RESIDUE	UNP P40927
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J	325	MSE	MET	MODIFIED RESIDUE	UNP P40927
J	327	MSE	MET	MODIFIED RESIDUE	UNP P40927
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J	374	MSE	MET	MODIFIED RESIDUE	UNP P40927
J	407	MSE	MET	MODIFIED RESIDUE	UNP P40927
J	577	MSE	MET	MODIFIED RESIDUE	UNP P40927
K	38	MSE	MET	MODIFIED RESIDUE	UNP P40927
K	86	MSE	MET	MODIFIED RESIDUE	UNP P40927
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K	577	MSE	MET	MODIFIED RESIDUE	UNP P40927
L	38	MSE	MET	MODIFIED RESIDUE	UNP P40927
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L	327	MSE	MET	MODIFIED RESIDUE	UNP P40927
L	343	MSE	MET	MODIFIED RESIDUE	UNP P40927
L	374	MSE	MET	MODIFIED RESIDUE	UNP P40927
L	407	MSE	MET	MODIFIED RESIDUE	UNP P40927
L	577	MSE	MET	MODIFIED RESIDUE	UNP P40927

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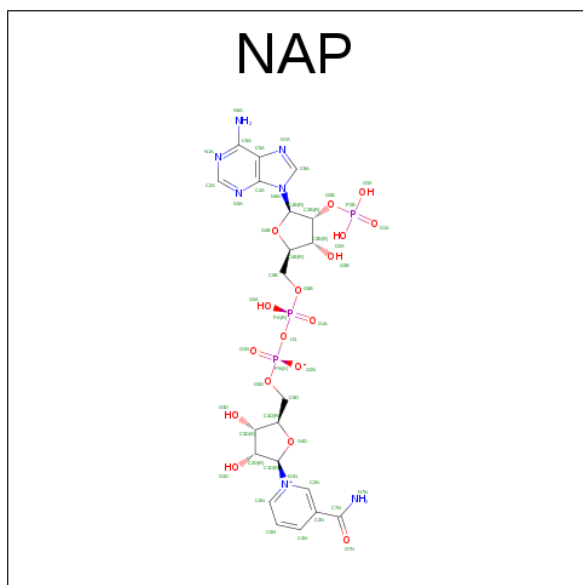
Chain	Residue	Modelled	Actual	Comment	Reference
M	38	MSE	MET	MODIFIED RESIDUE	UNP P40927
M	86	MSE	MET	MODIFIED RESIDUE	UNP P40927
M	108	MSE	MET	MODIFIED RESIDUE	UNP P40927
M	146	MSE	MET	MODIFIED RESIDUE	UNP P40927
M	177	MSE	MET	MODIFIED RESIDUE	UNP P40927
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M	407	MSE	MET	MODIFIED RESIDUE	UNP P40927
M	577	MSE	MET	MODIFIED RESIDUE	UNP P40927
N	38	MSE	MET	MODIFIED RESIDUE	UNP P40927
N	86	MSE	MET	MODIFIED RESIDUE	UNP P40927
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N	407	MSE	MET	MODIFIED RESIDUE	UNP P40927
N	577	MSE	MET	MODIFIED RESIDUE	UNP P40927
O	38	MSE	MET	MODIFIED RESIDUE	UNP P40927
O	86	MSE	MET	MODIFIED RESIDUE	UNP P40927
O	108	MSE	MET	MODIFIED RESIDUE	UNP P40927
O	146	MSE	MET	MODIFIED RESIDUE	UNP P40927
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O	325	MSE	MET	MODIFIED RESIDUE	UNP P40927
O	327	MSE	MET	MODIFIED RESIDUE	UNP P40927
O	343	MSE	MET	MODIFIED RESIDUE	UNP P40927
O	374	MSE	MET	MODIFIED RESIDUE	UNP P40927
O	407	MSE	MET	MODIFIED RESIDUE	UNP P40927
O	577	MSE	MET	MODIFIED RESIDUE	UNP P40927

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Chain	Residue	Modelled	Actual	Comment	Reference
P	38	MSE	MET	MODIFIED RESIDUE	UNP P40927
P	86	MSE	MET	MODIFIED RESIDUE	UNP P40927
P	108	MSE	MET	MODIFIED RESIDUE	UNP P40927
P	146	MSE	MET	MODIFIED RESIDUE	UNP P40927
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P	325	MSE	MET	MODIFIED RESIDUE	UNP P40927
P	327	MSE	MET	MODIFIED RESIDUE	UNP P40927
P	343	MSE	MET	MODIFIED RESIDUE	UNP P40927
P	374	MSE	MET	MODIFIED RESIDUE	UNP P40927
P	407	MSE	MET	MODIFIED RESIDUE	UNP P40927
P	577	MSE	MET	MODIFIED RESIDUE	UNP P40927

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



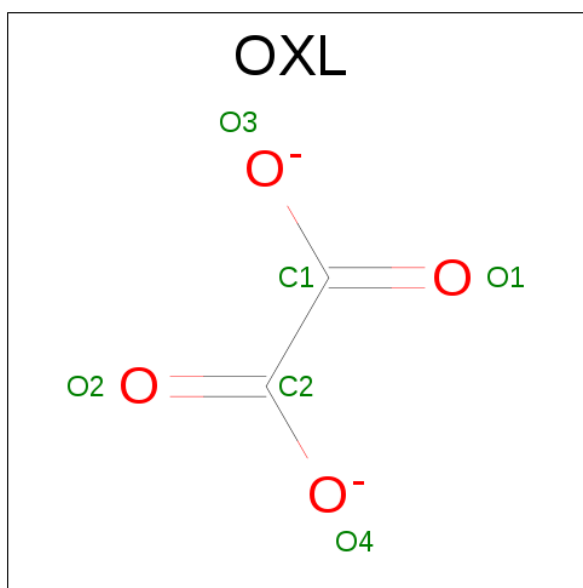
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	B	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	C	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	D	1	Total 48	C 21	N 7	O 17	P 3	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	H	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	I	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	J	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	K	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	L	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	M	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	N	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	O	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	P	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is OXALATE ION (three-letter code: OXL) (formula: C_2O_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 2 4	0	0
3	B	1	Total C O 6 2 4	0	0
3	C	1	Total C O 6 2 4	0	0
3	D	1	Total C O 6 2 4	0	0
3	E	1	Total C O 6 2 4	0	0
3	F	1	Total C O 6 2 4	0	0
3	G	1	Total C O 6 2 4	0	0
3	H	1	Total C O 6 2 4	0	0
3	I	1	Total C O 6 2 4	0	0
3	J	1	Total C O 6 2 4	0	0
3	K	1	Total C O 6 2 4	0	0
3	L	1	Total C O 6 2 4	0	0
3	M	1	Total C O 6 2 4	0	0
3	N	1	Total C O 6 2 4	0	0
3	O	1	Total C O 6 2 4	0	0
3	P	1	Total C O 6 2 4	0	0

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	P	1	Total Mn 1 1	0	0
4	G	1	Total Mn 1 1	0	0
4	J	1	Total Mn 1 1	0	0
4	D	1	Total Mn 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	K	1	Total 1	Mn 1	0	0
4	E	1	Total 1	Mn 1	0	0
4	H	1	Total 1	Mn 1	0	0
4	B	1	Total 1	Mn 1	0	0
4	I	1	Total 1	Mn 1	0	0
4	C	1	Total 1	Mn 1	0	0
4	A	1	Total 1	Mn 1	0	0
4	N	1	Total 1	Mn 1	0	0
4	O	1	Total 1	Mn 1	0	0
4	L	1	Total 1	Mn 1	0	0
4	F	1	Total 1	Mn 1	0	0
4	M	1	Total 1	Mn 1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	P	3	Total 3	Cl 3	0	0
5	G	1	Total 1	Cl 1	0	0
5	J	2	Total 2	Cl 2	0	0
5	K	1	Total 1	Cl 1	0	0
5	E	3	Total 3	Cl 3	0	0
5	H	1	Total 1	Cl 1	0	0
5	B	1	Total 1	Cl 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	5	Total 5	Cl 5	0	0
5	C	4	Total 4	Cl 4	0	0
5	N	2	Total 2	Cl 2	0	0
5	O	4	Total 4	Cl 4	0	0
5	L	1	Total 1	Cl 1	0	0
5	F	2	Total 2	Cl 2	0	0
5	M	3	Total 3	Cl 3	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	P	5	Total 5	Na 5	0	0
6	G	1	Total 1	Na 1	0	0
6	J	2	Total 2	Na 2	0	0
6	D	2	Total 2	Na 2	0	0
6	K	1	Total 1	Na 1	0	0
6	H	5	Total 5	Na 5	0	0
6	I	2	Total 2	Na 2	0	0
6	C	4	Total 4	Na 4	0	0
6	N	1	Total 1	Na 1	0	0
6	O	4	Total 4	Na 4	0	0
6	L	1	Total 1	Na 1	0	0
6	F	2	Total 2	Na 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	M	6	Total	Na	0	0
			6	6		

- Molecule 7 is water.

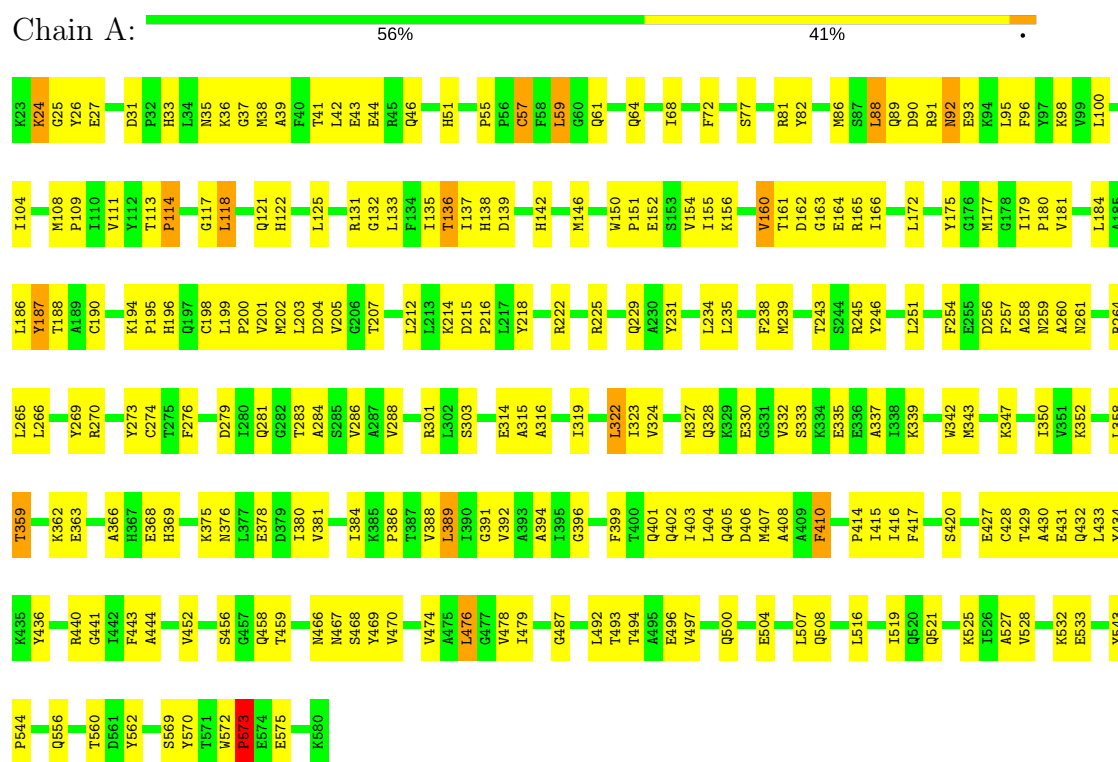
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	35	Total	O	0	0
			35	35		
7	B	42	Total	O	0	0
			42	42		
7	C	77	Total	O	0	0
			77	77		
7	D	49	Total	O	0	0
			49	49		
7	E	58	Total	O	0	0
			58	58		
7	F	78	Total	O	0	0
			78	78		
7	G	65	Total	O	0	0
			65	65		
7	H	77	Total	O	0	0
			77	77		
7	I	80	Total	O	0	0
			80	80		
7	J	63	Total	O	0	0
			63	63		
7	K	41	Total	O	0	0
			41	41		
7	L	75	Total	O	0	0
			75	75		
7	M	81	Total	O	0	0
			81	81		
7	N	71	Total	O	0	0
			71	71		
7	O	78	Total	O	0	0
			78	78		
7	P	79	Total	O	0	0
			79	79		

3 Residue-property plots

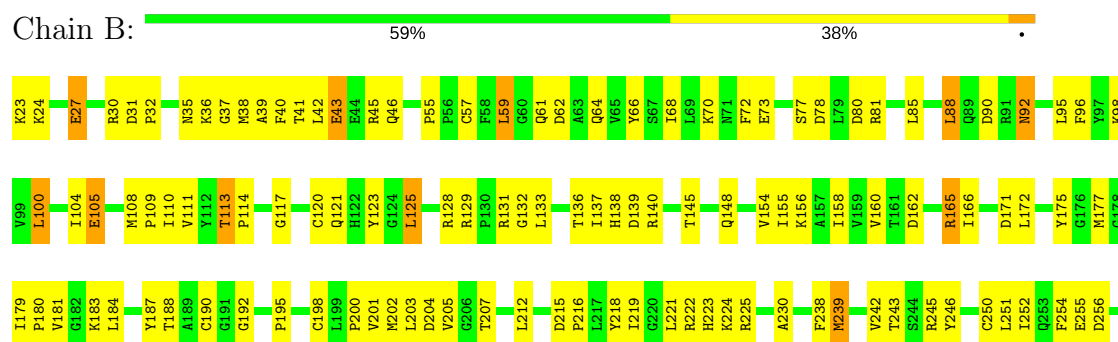
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

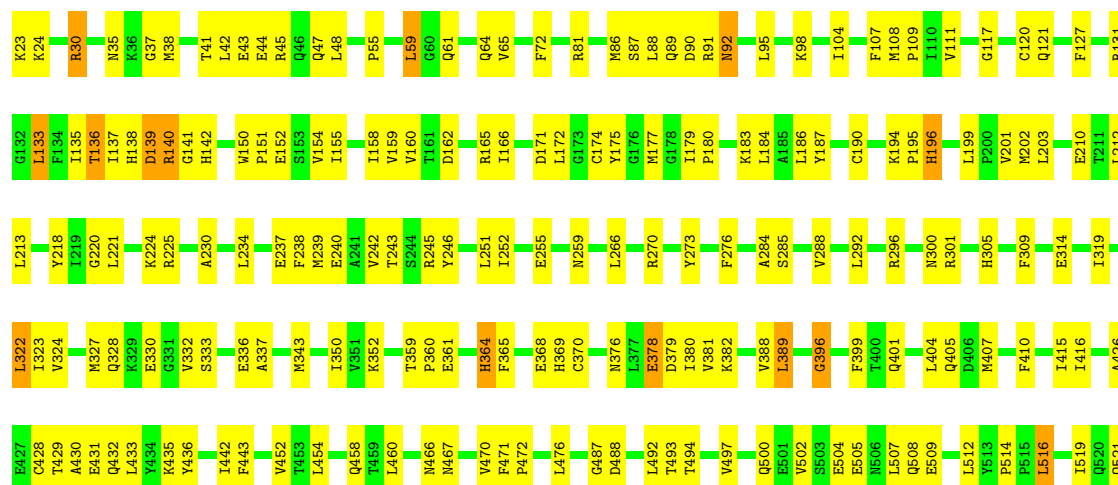
Note EDS was not executed.

• Molecule 1: MALIC ENZYME



• Molecule 1: MALIC ENZYME

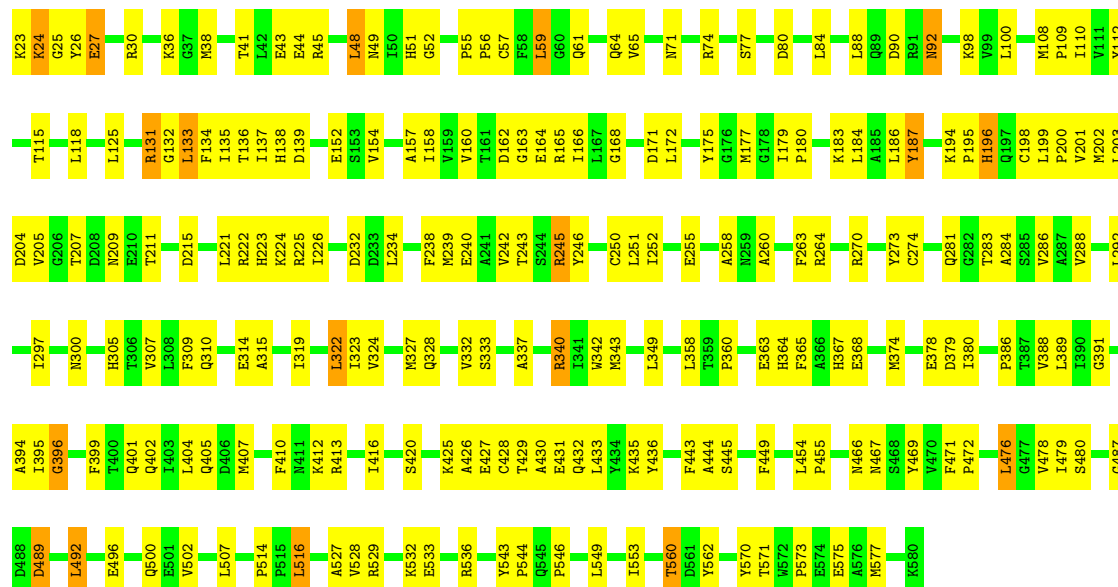






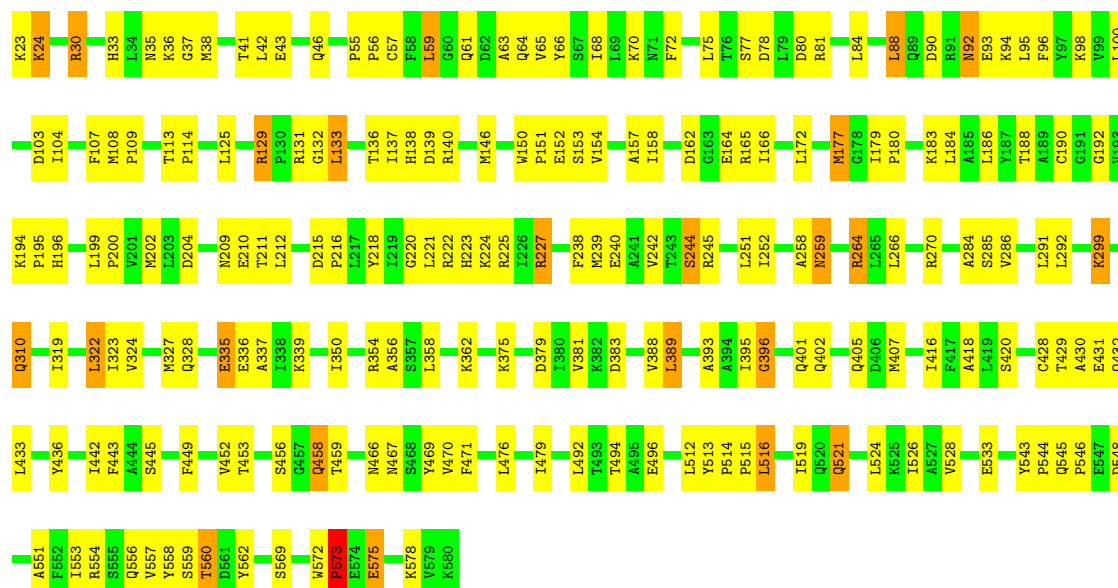
• Molecule 1: MALIC ENZYME

Chain E: 60% 36%



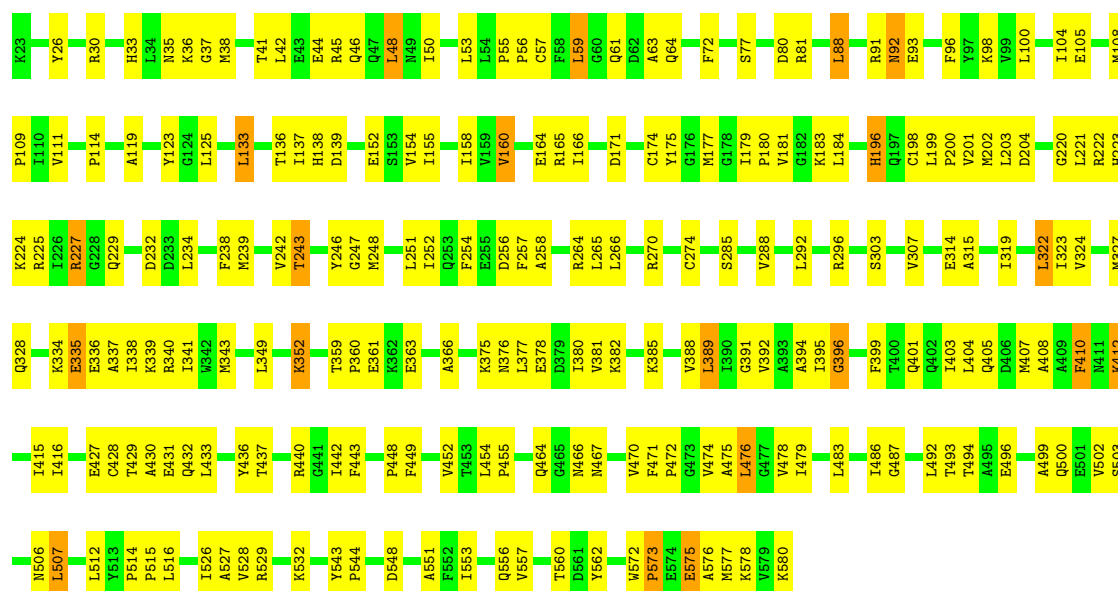
• Molecule 1: MALIC ENZYME

Chain F: 63% 33%



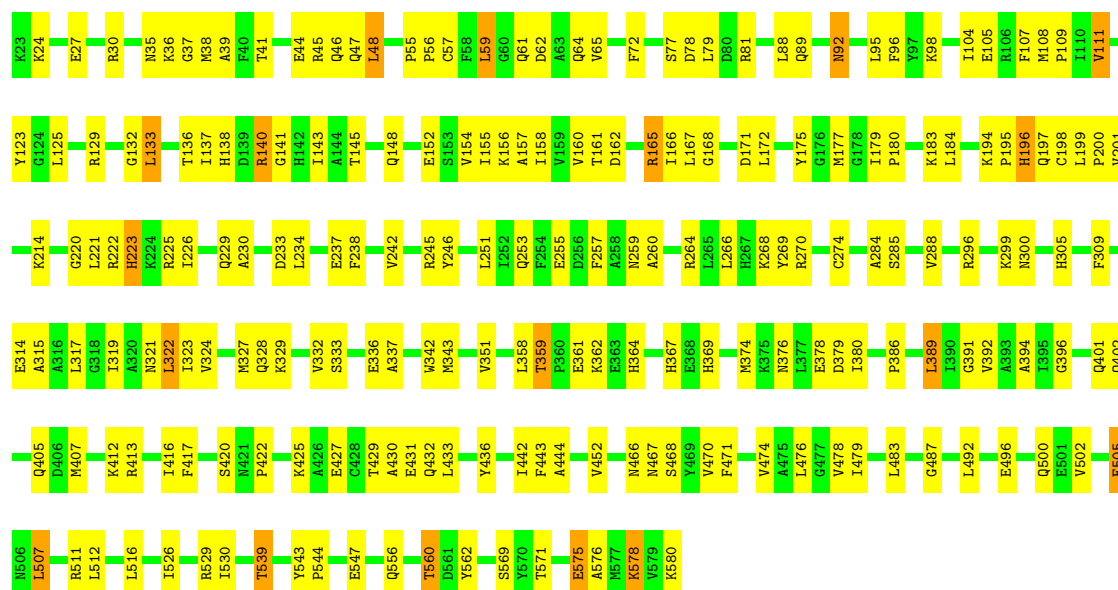
• Molecule 1: MALIC ENZYME

Chain G: 60% 36%



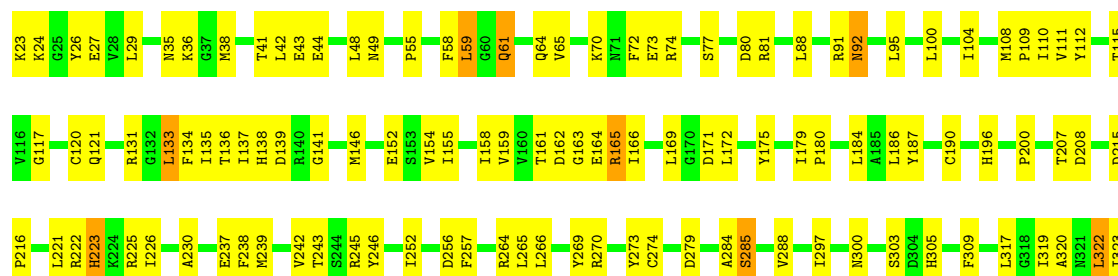
• Molecule 1: MALIC ENZYME

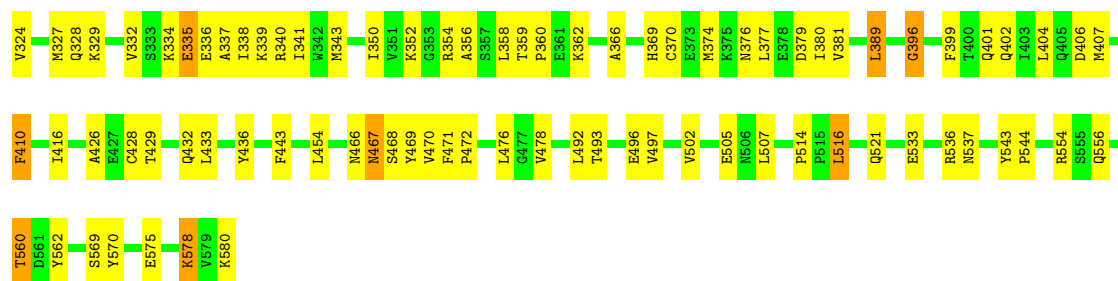
Chain H: 62% 35%



• Molecule 1: MALIC ENZYME

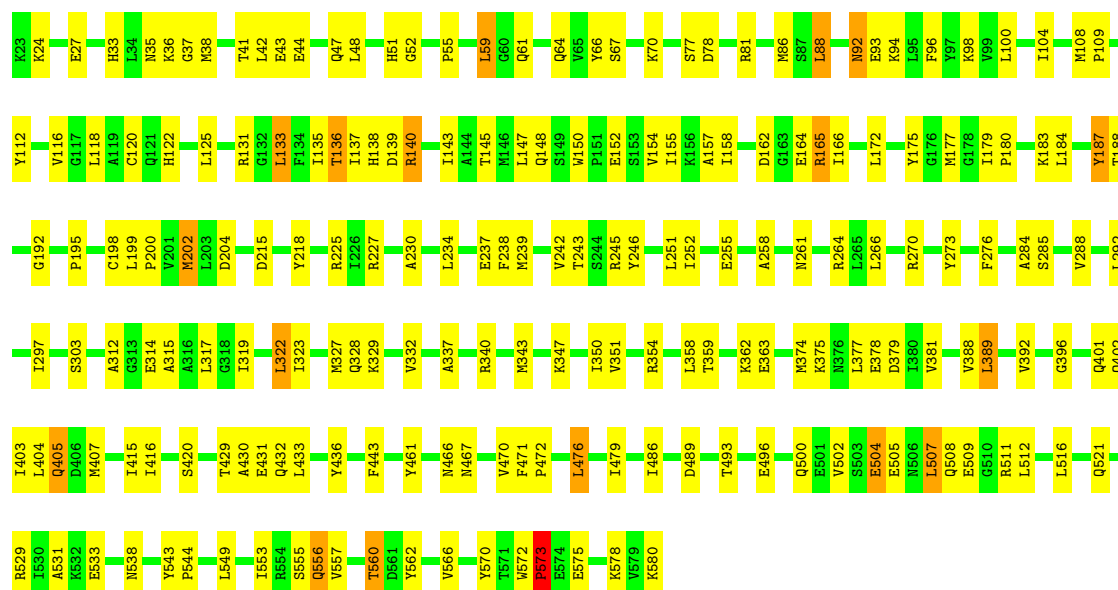
Chain I: 64% 33%





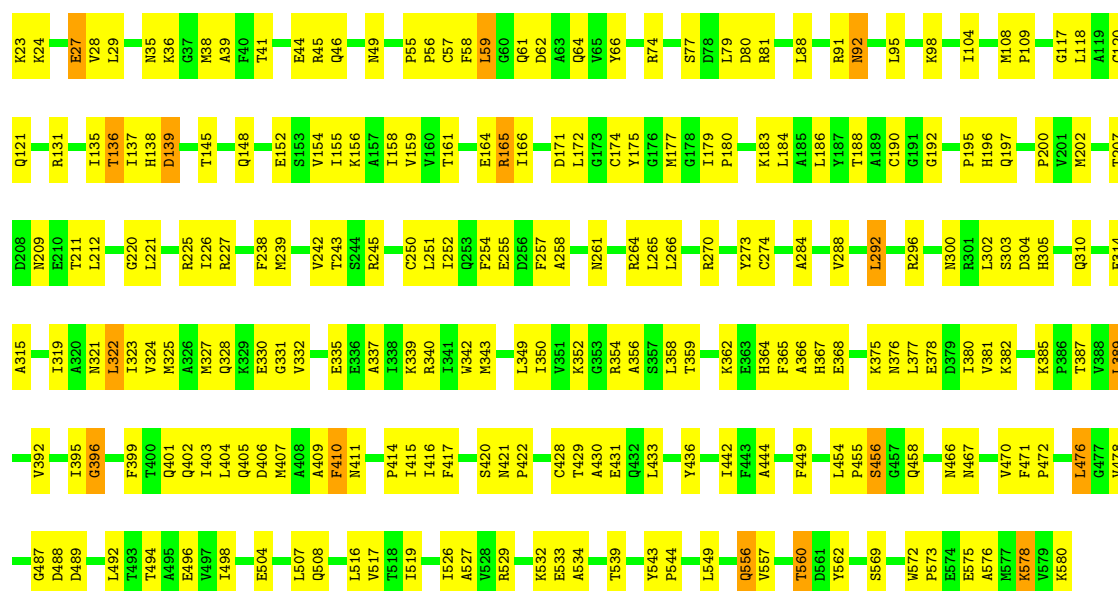
• Molecule 1: MALIC ENZYME

Chain J: 64% 33%

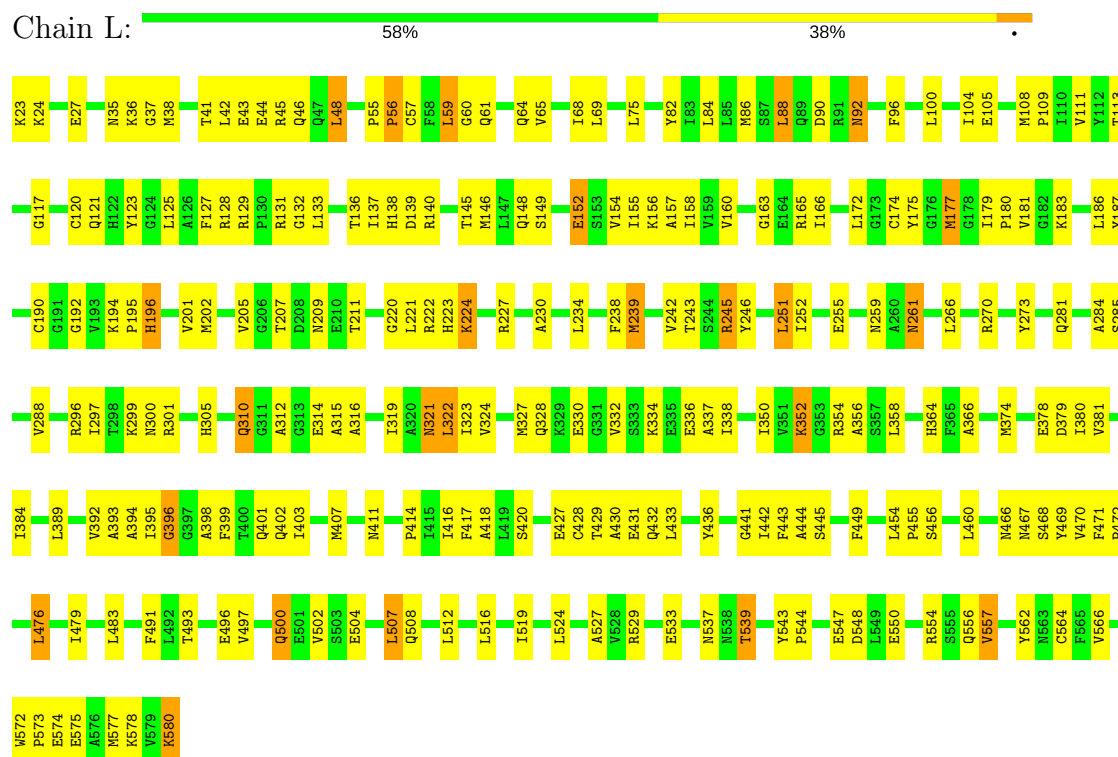


• Molecule 1: MALIC ENZYME

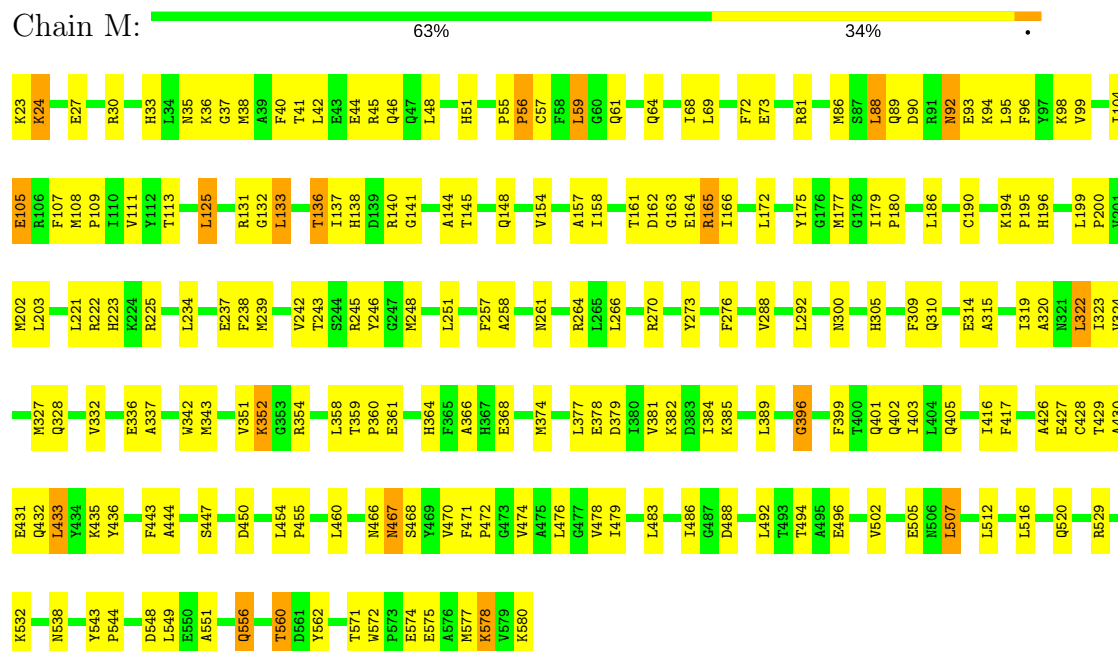
Chain K: 58% 39%



- Molecule 1: MALIC ENZYME

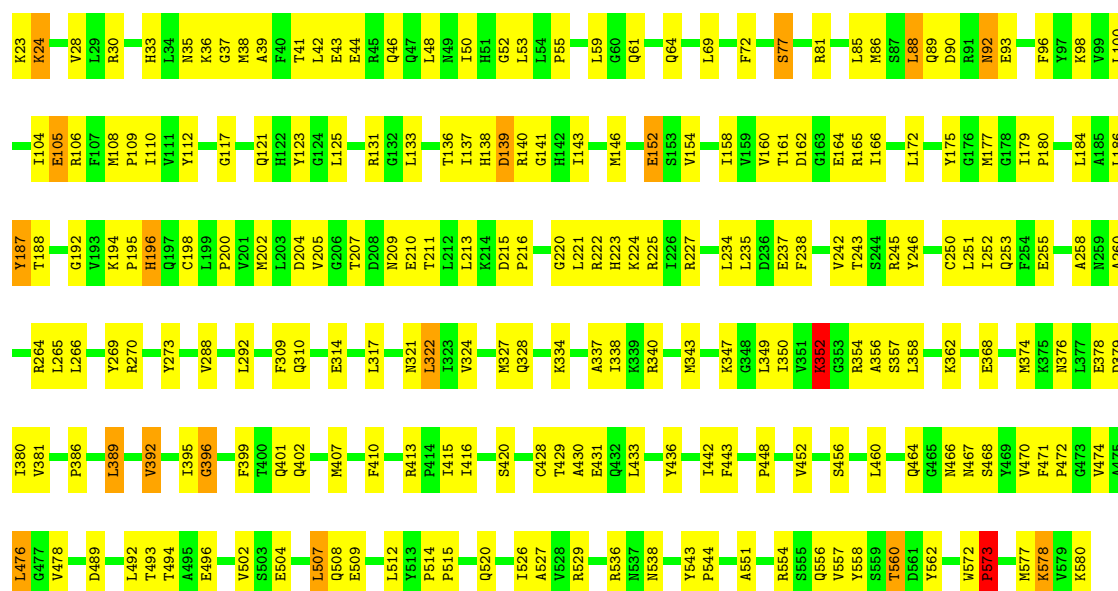


- Molecule 1: MALIC ENZYME



- Molecule 1: MALIC ENZYME





I319	T429	P544
A430	A430	R554
E431	E431	S555
Q432	Q432	Q556
L433	L433	V557
K327	E438	Y558
V332	F443	S559
E336	L454	T560
A337	P455	D561
R340	L460	Y562
T341	N466	V566
W342	N467	W572
I350	S468	P573
L358	F471	E574
K362	P472	E575
E363	G473	K578
H364	L476	V579
H367	G477	K580
V478	V478	
K374	G487	
K375	L492	
N376	T493	
D379	E496	
I380	V497	
V381	Q500	
K385	E501	
V388	V502	
L389	S503	
G396	E504	
F399	L507	
T400	Q508	
Q401	L516	
Q402	I519	
I403	Q520	
L404	Q521	
Q405	L524	
D406	A527	
H407	V528	
F410	R529	
N411	I530	
I415	E533	
I416	Y543	
A426		
E427		
C428		

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	124.15Å 140.86Å 167.08Å 90.05° 87.16° 75.63°	Depositor
Resolution (Å)	10.00 – 2.50	Depositor
% Data completeness (in resolution range)	83.0 (10.00-2.50)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.210 , 0.256	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	71519	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

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: OXL, NA, NAP, MN, CL

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	0.39	0/4420	0.61	0/5962
1	B	0.38	0/4420	0.61	0/5962
1	C	0.40	0/4420	0.62	1/5962 (0.0%)
1	D	0.40	0/4420	0.62	0/5962
1	E	0.38	0/4420	0.61	0/5962
1	F	0.40	0/4420	0.63	1/5962 (0.0%)
1	G	0.39	0/4420	0.62	0/5962
1	H	0.41	0/4420	0.62	0/5962
1	I	0.40	0/4420	0.63	0/5962
1	J	0.40	0/4420	0.61	0/5962
1	K	0.39	0/4420	0.61	0/5962
1	L	0.39	0/4420	0.62	0/5962
1	M	0.41	0/4420	0.63	0/5962
1	N	0.40	0/4420	0.63	1/5962 (0.0%)
1	O	0.39	0/4420	0.62	0/5962
1	P	0.39	0/4421	0.62	0/5962
All	All	0.39	0/70721	0.62	3/95392 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	251	LEU	CA-CB-CG	5.19	127.24	115.30
1	F	310	GLN	N-CA-C	-5.11	97.21	111.00
1	N	352	LYS	N-CA-C	5.09	124.75	111.00

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	4345	0	4366	230	0
1	B	4345	0	4366	216	0
1	C	4345	0	4366	219	0
1	D	4345	0	4366	196	0
1	E	4345	0	4366	189	0
1	F	4345	0	4366	193	0
1	G	4345	0	4366	197	0
1	H	4345	0	4366	178	0
1	I	4345	0	4366	181	0
1	J	4345	0	4366	200	0
1	K	4345	0	4366	208	0
1	L	4345	0	4366	227	0
1	M	4345	0	4366	188	0
1	N	4345	0	4366	207	0
1	O	4345	0	4366	226	0
1	P	4346	0	4366	194	0
2	A	48	0	25	4	0
2	B	48	0	25	4	0
2	C	48	0	25	2	0
2	D	48	0	25	2	0
2	E	48	0	25	3	0
2	F	48	0	25	2	0
2	G	48	0	25	3	0
2	H	48	0	25	3	0
2	I	48	0	25	3	0
2	J	48	0	25	4	0
2	K	48	0	25	5	0
2	L	48	0	25	5	0
2	M	48	0	25	3	0
2	N	48	0	25	3	0
2	O	48	0	25	2	0
2	P	48	0	25	1	0
3	A	6	0	0	1	0
3	B	6	0	0	1	0
3	C	6	0	0	3	0
3	D	6	0	0	2	0
3	E	6	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	6	0	0	1	0
3	G	6	0	0	1	0
3	H	6	0	0	1	0
3	I	6	0	0	0	0
3	J	6	0	0	1	0
3	K	6	0	0	1	0
3	L	6	0	0	1	0
3	M	6	0	0	0	0
3	N	6	0	0	1	0
3	O	6	0	0	0	0
3	P	6	0	0	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
4	M	1	0	0	0	0
4	N	1	0	0	0	0
4	O	1	0	0	0	0
4	P	1	0	0	0	0
5	B	1	0	0	0	0
5	C	4	0	0	1	0
5	E	3	0	0	1	0
5	F	2	0	0	1	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	5	0	0	1	0
5	J	2	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
5	M	3	0	0	1	0
5	N	2	0	0	1	0
5	O	4	0	0	3	0
5	P	3	0	0	3	0
6	C	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	2	0	0	0	0
6	F	2	0	0	0	0
6	G	1	0	0	0	0
6	H	5	0	0	0	0
6	I	2	0	0	0	0
6	J	2	0	0	0	0
6	K	1	0	0	0	0
6	L	1	0	0	0	0
6	M	6	0	0	0	0
6	N	1	0	0	0	0
6	O	4	0	0	0	0
6	P	5	0	0	0	0
7	A	35	0	0	6	0
7	B	42	0	0	6	0
7	C	77	0	0	7	0
7	D	49	0	0	2	0
7	E	58	0	0	5	0
7	F	78	0	0	6	0
7	G	65	0	0	6	0
7	H	77	0	0	7	0
7	I	80	0	0	7	0
7	J	63	0	0	3	0
7	K	41	0	0	5	0
7	L	75	0	0	7	0
7	M	81	0	0	7	0
7	N	71	0	0	7	0
7	O	78	0	0	8	0
7	P	79	0	0	4	0
All	All	71519	0	70256	3151	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 22.

The worst 5 of 3151 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:H:136:THR:HG22	1:H:138:HIS:H	1.08	1.17
1:N:136:THR:HG22	1:N:138:HIS:H	1.04	1.17
1:K:98:LYS:HD3	1:K:560:THR:HG21	1.30	1.14
1:F:136:THR:HG22	1:F:138:HIS:H	1.10	1.13
1:B:136:THR:HG22	1:B:138:HIS:H	1.06	1.13

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	553/555 (100%)	524 (95%)	23 (4%)	6 (1%)	17	29
1	B	553/555 (100%)	530 (96%)	21 (4%)	2 (0%)	38	59
1	C	553/555 (100%)	530 (96%)	21 (4%)	2 (0%)	38	59
1	D	553/555 (100%)	530 (96%)	21 (4%)	2 (0%)	38	59
1	E	553/555 (100%)	530 (96%)	22 (4%)	1 (0%)	51	73
1	F	553/555 (100%)	529 (96%)	22 (4%)	2 (0%)	38	59
1	G	553/555 (100%)	531 (96%)	19 (3%)	3 (0%)	32	53
1	H	553/555 (100%)	534 (97%)	16 (3%)	3 (0%)	32	53
1	I	553/555 (100%)	535 (97%)	17 (3%)	1 (0%)	51	73
1	J	553/555 (100%)	531 (96%)	19 (3%)	3 (0%)	32	53
1	K	553/555 (100%)	524 (95%)	27 (5%)	2 (0%)	38	59
1	L	553/555 (100%)	534 (97%)	14 (2%)	5 (1%)	20	36
1	M	553/555 (100%)	528 (96%)	23 (4%)	2 (0%)	38	59
1	N	553/555 (100%)	528 (96%)	21 (4%)	4 (1%)	25	43
1	O	553/555 (100%)	531 (96%)	18 (3%)	4 (1%)	25	43
1	P	553/555 (100%)	532 (96%)	18 (3%)	3 (0%)	32	53
All	All	8848/8880 (100%)	8481 (96%)	322 (4%)	45 (0%)	32	53

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	396	GLY
1	A	573	PRO
1	B	396	GLY
1	C	396	GLY

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Mol	Chain	Res	Type
1	D	396	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	467/453 (103%)	438 (94%)	29 (6%)	21	39
1	B	467/453 (103%)	438 (94%)	29 (6%)	21	39
1	C	467/453 (103%)	437 (94%)	30 (6%)	20	38
1	D	467/453 (103%)	439 (94%)	28 (6%)	22	41
1	E	467/453 (103%)	431 (92%)	36 (8%)	15	28
1	F	467/453 (103%)	434 (93%)	33 (7%)	17	32
1	G	467/453 (103%)	441 (94%)	26 (6%)	25	45
1	H	467/453 (103%)	437 (94%)	30 (6%)	20	38
1	I	467/453 (103%)	439 (94%)	28 (6%)	22	41
1	J	467/453 (103%)	437 (94%)	30 (6%)	20	38
1	K	467/453 (103%)	443 (95%)	24 (5%)	28	50
1	L	467/453 (103%)	437 (94%)	30 (6%)	20	38
1	M	467/453 (103%)	432 (92%)	35 (8%)	16	29
1	N	467/453 (103%)	443 (95%)	24 (5%)	28	50
1	O	467/453 (103%)	437 (94%)	30 (6%)	20	38
1	P	467/453 (103%)	430 (92%)	37 (8%)	14	27
All	All	7472/7248 (103%)	6993 (94%)	479 (6%)	20	38

5 of 479 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	62	ASP
1	I	578	LYS
1	P	48	LEU
1	H	196	HIS

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Mol	Chain	Res	Type
1	I	59	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 286 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	92	ASN
1	I	467	ASN
1	O	405	GLN
1	H	271	ASN
1	H	545	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 117 ligands modelled in this entry, 85 are monoatomic - leaving 32 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAP	A	1581	-	44,52,52	1.70	10 (22%)	51,80,80	1.76	3 (5%)
3	OXL	A	1583	4	0,5,5	0.00	-	0,6,6	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAP	B	1581	-	44,52,52	1.56	10 (22%)	51,80,80	1.73	4 (7%)
3	OXL	B	1582	4	0,5,5	0.00	-	0,6,6	0.00	-
2	NAP	C	1581	-	44,52,52	1.65	7 (15%)	51,80,80	1.76	4 (7%)
3	OXL	C	1582	4	0,5,5	0.00	-	0,6,6	0.00	-
2	NAP	D	1581	-	44,52,52	1.60	9 (20%)	51,80,80	1.84	4 (7%)
3	OXL	D	1582	4,6	0,5,5	0.00	-	0,6,6	0.00	-
2	NAP	E	1581	-	44,52,52	1.67	9 (20%)	51,80,80	1.77	4 (7%)
3	OXL	E	1582	4	0,5,5	0.00	-	0,6,6	0.00	-
2	NAP	F	1581	-	44,52,52	1.60	8 (18%)	51,80,80	1.78	5 (9%)
3	OXL	F	1582	4	0,5,5	0.00	-	0,6,6	0.00	-
2	NAP	G	1581	-	44,52,52	1.58	6 (13%)	51,80,80	1.79	4 (7%)
3	OXL	G	1582	4	0,5,5	0.00	-	0,6,6	0.00	-
2	NAP	H	1581	-	44,52,52	1.62	9 (20%)	51,80,80	1.78	5 (9%)
3	OXL	H	1582	4	0,5,5	0.00	-	0,6,6	0.00	-
2	NAP	I	1581	-	44,52,52	1.71	11 (25%)	51,80,80	1.79	4 (7%)
3	OXL	I	1582	4	0,5,5	0.00	-	0,6,6	0.00	-
2	NAP	J	1581	-	44,52,52	1.62	8 (18%)	51,80,80	1.85	4 (7%)
3	OXL	J	1582	4	0,5,5	0.00	-	0,6,6	0.00	-
2	NAP	K	1581	-	44,52,52	1.68	8 (18%)	51,80,80	1.81	5 (9%)
3	OXL	K	1582	4	0,5,5	0.00	-	0,6,6	0.00	-
2	NAP	L	1581	-	44,52,52	1.77	11 (25%)	51,80,80	1.78	3 (5%)
3	OXL	L	1582	4	0,5,5	0.00	-	0,6,6	0.00	-
2	NAP	M	1581	-	44,52,52	1.55	8 (18%)	51,80,80	1.75	5 (9%)
3	OXL	M	1582	4	0,5,5	0.00	-	0,6,6	0.00	-
2	NAP	N	1581	-	44,52,52	1.70	9 (20%)	51,80,80	1.79	4 (7%)
3	OXL	N	1582	4	0,5,5	0.00	-	0,6,6	0.00	-
2	NAP	O	1581	-	44,52,52	1.62	9 (20%)	51,80,80	1.82	4 (7%)
3	OXL	O	1582	4	0,5,5	0.00	-	0,6,6	0.00	-
2	NAP	P	1581	-	44,52,52	1.56	10 (22%)	51,80,80	1.76	5 (9%)
3	OXL	P	1582	4	0,5,5	0.00	-	0,6,6	0.00	-

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	NAP	A	1581	-	-	0/27/67/67	0/5/5/5
3	OXL	A	1583	4	-	0/0/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	B	1581	-	-	0/27/67/67	0/5/5/5
3	OXL	B	1582	4	-	0/0/4/4	0/0/0/0
2	NAP	C	1581	-	-	0/27/67/67	0/5/5/5
3	OXL	C	1582	4	-	0/0/4/4	0/0/0/0
2	NAP	D	1581	-	-	0/27/67/67	0/5/5/5
3	OXL	D	1582	4,6	-	0/0/4/4	0/0/0/0
2	NAP	E	1581	-	-	0/27/67/67	0/5/5/5
3	OXL	E	1582	4	-	0/0/4/4	0/0/0/0
2	NAP	F	1581	-	-	0/27/67/67	0/5/5/5
3	OXL	F	1582	4	-	0/0/4/4	0/0/0/0
2	NAP	G	1581	-	-	0/27/67/67	0/5/5/5
3	OXL	G	1582	4	-	0/0/4/4	0/0/0/0
2	NAP	H	1581	-	-	0/27/67/67	0/5/5/5
3	OXL	H	1582	4	-	0/0/4/4	0/0/0/0
2	NAP	I	1581	-	-	0/27/67/67	0/5/5/5
3	OXL	I	1582	4	-	0/0/4/4	0/0/0/0
2	NAP	J	1581	-	-	0/27/67/67	0/5/5/5
3	OXL	J	1582	4	-	0/0/4/4	0/0/0/0
2	NAP	K	1581	-	-	0/27/67/67	0/5/5/5
3	OXL	K	1582	4	-	0/0/4/4	0/0/0/0
2	NAP	L	1581	-	-	0/27/67/67	0/5/5/5
3	OXL	L	1582	4	-	0/0/4/4	0/0/0/0
2	NAP	M	1581	-	-	0/27/67/67	0/5/5/5
3	OXL	M	1582	4	-	0/0/4/4	0/0/0/0
2	NAP	N	1581	-	-	0/27/67/67	0/5/5/5
3	OXL	N	1582	4	-	0/0/4/4	0/0/0/0
2	NAP	O	1581	-	-	0/27/67/67	0/5/5/5
3	OXL	O	1582	4	-	0/0/4/4	0/0/0/0
2	NAP	P	1581	-	-	0/27/67/67	0/5/5/5
3	OXL	P	1582	4	-	0/0/4/4	0/0/0/0

The worst 5 of 142 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1581	NAP	C5A-C4A	-3.46	1.32	1.40
2	J	1581	NAP	C5A-C4A	-3.34	1.33	1.40
2	P	1581	NAP	C5A-C4A	-3.31	1.33	1.40
2	F	1581	NAP	C5A-C4A	-3.30	1.33	1.40
2	F	1581	NAP	C2D-C1D	-3.24	1.48	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1581	NAP	N3A-C2A-N1A	-10.03	120.13	128.86
2	J	1581	NAP	N3A-C2A-N1A	-9.72	120.39	128.86
2	G	1581	NAP	N3A-C2A-N1A	-9.68	120.43	128.86
2	L	1581	NAP	N3A-C2A-N1A	-9.63	120.47	128.86
2	H	1581	NAP	N3A-C2A-N1A	-9.59	120.50	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

29 monomers are involved in 65 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1581	NAP	4	0
3	A	1583	OXL	1	0
2	B	1581	NAP	4	0
3	B	1582	OXL	1	0
2	C	1581	NAP	2	0
3	C	1582	OXL	3	0
2	D	1581	NAP	2	0
3	D	1582	OXL	2	0
2	E	1581	NAP	3	0
3	E	1582	OXL	1	0
2	F	1581	NAP	2	0
3	F	1582	OXL	1	0
2	G	1581	NAP	3	0
3	G	1582	OXL	1	0
2	H	1581	NAP	3	0
3	H	1582	OXL	1	0
2	I	1581	NAP	3	0
2	J	1581	NAP	4	0
3	J	1582	OXL	1	0
2	K	1581	NAP	5	0
3	K	1582	OXL	1	0
2	L	1581	NAP	5	0
3	L	1582	OXL	1	0
2	M	1581	NAP	3	0
2	N	1581	NAP	3	0
3	N	1582	OXL	1	0
2	O	1581	NAP	2	0
2	P	1581	NAP	1	0
3	P	1582	OXL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.